# SP-Wax: SLE thermodynamic modeling software for binary and multicomponent paraffinic systems

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# Abstract

The open-source software (SP-Wax) the for 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. Coutinho et al. thermodynamic model was primarily used and coded in SP-Wax. The developed simulation was, then, 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 exploitation of petroleum resources in harsh and deep-water environments. Such locations require long subsea pipelines for transporting hydrocarbons to Central Processing Platform (CPP), Floating Production Storage and Offloading (FPSO), from offshore to onshore facilities, etc. 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, a platform abandonment at the cost of $100 million occurred, due to a paraffin deposition problem [1–5]. Typical approaches of mitigating wax deposition problems in subsea pipelines are mechanical (“pigging”) and chemical approaches. The mechanical approach is mainly done by using a mechanical device (“pig”) to scrape any deposit from the pipes. The pig is placed inside the pipeline and pushed forward by production stream. Pigging should be performed while deposit is soft to prevent the pig from getting stuck in the pipe [3]. The chemical approach is generally performed by adding chemical products to crude oil. These chemicals are solvents, paraffin inhibitors, dispersants, etc. [6].

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It is important to note that both methods are expensive. Aside from operational point of view, deferring production (due to paraffin treatment) can be very costly (e.g. loss of twenty-five million dollars revenue for pigging subsea pipelines every seven days [7]). Three factors are responsible for determining the pigging frequency and the amount of chemical needed to mitigate wax deposition problems. These factors are deposit thickness, solid wax fraction [8] and carbon number distribution (CND) of the deposit [9]. Current paraffin deposition models determine the deposit’s thickness and solid wax fraction based on heat and mass transfer calculations [4,9–11]. The mass transfer calculation section requires a reliable thermodynamic model to accurately determine the deposit composition. This software provides an open-source thermodynamics package for the paraffin modeling in wax deposition and other related fields. Furthermore, the studies on multiphase flow paraffin depositions [9,12–14] should benefit from this open-source high performance software package. In complex multiphase flow conditions, an accurate thermodynamic model of wax is required for the model development of paraffin deposition phenomenon

# Software Description

In this section, theoretical framework of the SP-Wax software is presented. SP-Wax is based on thermodynamic model of Coutinho and co-workers [15–22] and other literature [10,23–40]. We chose Coutinho model because it is superior to other models in terms of describing the non-ideality of liquid and solid phases [15–22]. In SP-Wax, the governing equations [24] are solved for non-ideal paraffinic solutions. The following governing equation relates ith carbon number’s equilibrium constant () to enthalpy of fusion (), enthalpy of solid-phase transition (), temperature of fusion (), temperature of solid-phase transition () and the difference between specific heat capacity in liquid and solid phase () using activity coefficients of liquid and solid phases ().

|  |  |
| --- | --- |
|  | (1) |
|  | (2) |

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

The solid mole fraction () is then calculated based on equilibrium constant values and input n-alkane mole composition data () from [30]:

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

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

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

Researchers have used different models to express activity coefficients to quantify non-idealities of solid and liquid phases. Liquid phase non-ideality is mainly due to different molecular shapes and sizes. In SP-Wax, we used the Entropic free-volume model to express activity coefficient of liquid phase as [18]:

|  |  |
| --- | --- |
| Where and are combinatorial contribution and composition fraction parameters respectively. then can be expressed as follows: | (6) |
|  | (7) |

The parameter was modeled differently by different researchers. SP-Wax used the suggestion from Coutinho et al. [18] to calculate from the Entropic-free-volume (E-FV2/3) model as follows:

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

Where, and are molar and Van der Waals volume parameters respectively.

This E-FV2/3 model was selected, because it gives a more accurate prediction for the liquid phase non-ideality [18].

The molar volume ) is calculated through DIPPR correlations [27] for carbon numbers () larger than seven and smaller than twenty (). GCVOL group contribution method [29] was used for the rest of the carbon number components ( or ). Van der Waals volumes ) for different carbon number components were calculated from Bondi et al. [28].

The solid phase activity coefficient of each component, , is needed for calculation in Eq. (1). However, researchers have difficulties to accurately quantify the non-ideal behavior of the solid-phase. For solid-phase activity coefficient, Coutinho et al. [17,20] suggested two different approaches, including UNIQUAC and Wilson models. The Wilson model considers only one solid phase and requires simpler numerical scheme. Furthermore, Coutinho et al. [20] compared UNIQUAC and Wilson models versus several experimental data and showed that both models result in very similar predictions. Therefore, Wilson model [17] was selected for expressing the activity coefficients of solid-phase in SP-Wax software. The Wilson model is as follows:

|  |  |
| --- | --- |
| Where is the major binary interaction energy parameter in Wilson equationand is calculated based on minor binary interaction energy parameter between similar and different carbon number components ( and ) | (9) |
|  | (10) | |
|  | (11) | |
| Where is a correction factor and is heat of sublimation and it is calculated by | (12) | |
|  | (13) | |

Enthalpies of fusion and solid-phase transition () were calculated using correlations proposed by Coutinho et al. [19]. Extension of Pitzer CSP model [39] was used to calculate enthalpies of vaporization (). For more details, please refer to developer’s manual.

The is the interaction energy parameter which, typically, quantifies interaction energy between short and long n-alkane molecules. The general assumption [21] is to have the interaction energy between a long and a short n-alkane (), the same as the interaction between two short n-alkanes ()or . However, if molecules are too different in size, they can bend over further and cause more interactions. This invalidates the assumption of . Therefore, the correction factor has been introduced to account for such abnormalities. This correction factor ,, is important for the correct prediction of solid-phase composition and precipitation curve. However, it has not been evaluated thoroughly in the literature. Yang et al. [38], Coutinho et al. [21], and Fleming et al.[35] model this differently. Yet, all of these models for either contain an adjustment parameter or additional empirical correlations to evaluate . The criterion used for selecting the correlation of in SP-Wax is that the selected correlation should allow a reasonable match of the prediction with the experimental data. We found that Coutinho et al. [21] type model allows a proper match. Thus, Coutinho et al. [21] approach is selected for SP-Wax.

This approach (Coutinho et al. [20]), relates enthalpies of sublimation () to In their paper [20], 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 that was used by Coutinho et al. [20] (shown below). This worked well for all multicomponent systems.

|  |  |
| --- | --- |
|  | (14) |
|  | (15) |

In the above formula, the parameter “” is needed to be adjusted to tune the precipitation curve prediction to experimental precipitation data. Among three of analyzed oil samples (Rittirong [31], Panacharoensawad [10], Zheng et al.[34]), 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 Fleming et al.[35] case, the solution only contained n-alkanes. A smaller correction factor was needed () for the best match to the experimental data. Based on these four analyzed oil samples, we provided a general suggestion for the value of “”. Therefore, the user has a suggested value (shown in Eq (16) – (18)) for the parameter “” when experimental precipitation data are not available. Yet, in the case where the experimental data are available, the following closure relationship for a parameter “” is suggested.

|  |  |
| --- | --- |
|  | (16) |
|  | (17) |
| Where is the weight fraction of n-alkanes in the total system and should be provided by the user. | (18) |

We compared experimental data of four multicomponent systems and adjusted for all of them. For three oil compositions where n-alkane system weight fractions were less than 0.15, was calculated to be . However, for the case where only n-alkanes were present (), a very small minimum adjustment ( close to zero) was needed.

The above set of equations was solved iteratively in SP-Wax to predict the phase equilibria of paraffin. In addition to the software validation with the phase equilibrium data, SP-Wax was also used to analyze the composition of wax deposits. This was done by assuming that deposit composition can be approximated from the temperature information at a certain instance. The purpose of this analysis is not to replace the compositional wax deposition model, such as the one from Zheng et al.[34]. 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 time instance is available. Moreover, this wax deposit analysis proves that solid-phase composition prediction from our developed software is reliable. Interestingly, SP-Wax approximation matches reasonably well with the experimental data of Rittirong [31] and Panacharoensawad’s [10] single-phase wax deposition cases (See Illustrative Example section). In part, this is because the deposit temperature value was obtained from Rittirong [31] and Panacharoensawad’s [10] calculations that have already accounted for the deposit thickness and the solid fraction of the deposit. Nevertheless, their heat transfer calculations are not sensitive to the deposit composition (only sensitive to the deposit solid fraction), but the composition prediction can still be performed by SP-Wax. Users are referred to Rittrong [31] and Panacharoensawad [10] for more information on the deposit temperature calculations.

## 2.1 Software architecture

SP-Wax consists of the core calculation and Windows Form user interface. C++ was used for the core calculation with OpenMP parallel computation technique to maximize the calculation speed. C# GUI was used to create a front-end for users. C# GUI takes the user inputs, allows save and load operations, and shows the result after the calculation is finished. This improves the reusability of the program for technical and non-technical users. C# creates short text files as inputs for C++ calculations. It, then, reads the results and plots them in a graphical format. The C++ kernel calculates the solid and liquid phase compositions of the system by solving the SLE governing equation Eq. (1). Pre-calculated equilibrium constants, , are used to solve for precipitated solid mole fraction) and compositions of both phases( and ). The pre-calculated are used as the initial guess values for to ensure the numerical stability of the software. Then, the activity coefficients, , are calculated based on Eq. (6) and Eq. (9). These are used to calculate new values of . The newly obtained values will be considered as initial guesses to calculate values of the next point. 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 manual of the software. The following flowchart is a summary of SP-Wax thermodynamic model for 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 precipitation curve and WAT based on provided input data (SPWaxPrecipitation.cpp). SP-Wax calculates weight fractions of precipitated wax in total fluid at certain temperatures and plots them. The generated curve is called precipitation curve and it is used extensively in wax deposition simulations [4,10,11,31,40]. SP-Wax allows users to plot experimental solid fraction points versus predicted precipitation curve for adjustment of correction factor coefficient in the thermodynamic model (Eq. (14)). Moreover, solid-phase composition can be plotted at any temperature within the given range using a track-bar. This provides a quick tool for users to compare carbon number distributions of solid-phase at different temperatures.

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). By this program option, a user can choose the desired output 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 values are calculated by SPWaxKInitialization.cpp. This C++ source file takes input information of the oil samples and calculates equilibrium constant values at every half temperature () ranging from to WAT. Then, calculated , values are reported to a text file which will be accessed as initial values for equilibrium constants for calculating SLE properties of the solution at any desired temperature. By this method, we eliminated the convergence problem near WAT.

The third multicomponent simulation option enables the user to plot relative concentration gradients of all carbon numbers. In this graph, the smallest carbon number with positive relative concentration gradient is 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 following picture shows SP-Wax software interface for multicomponent systems.

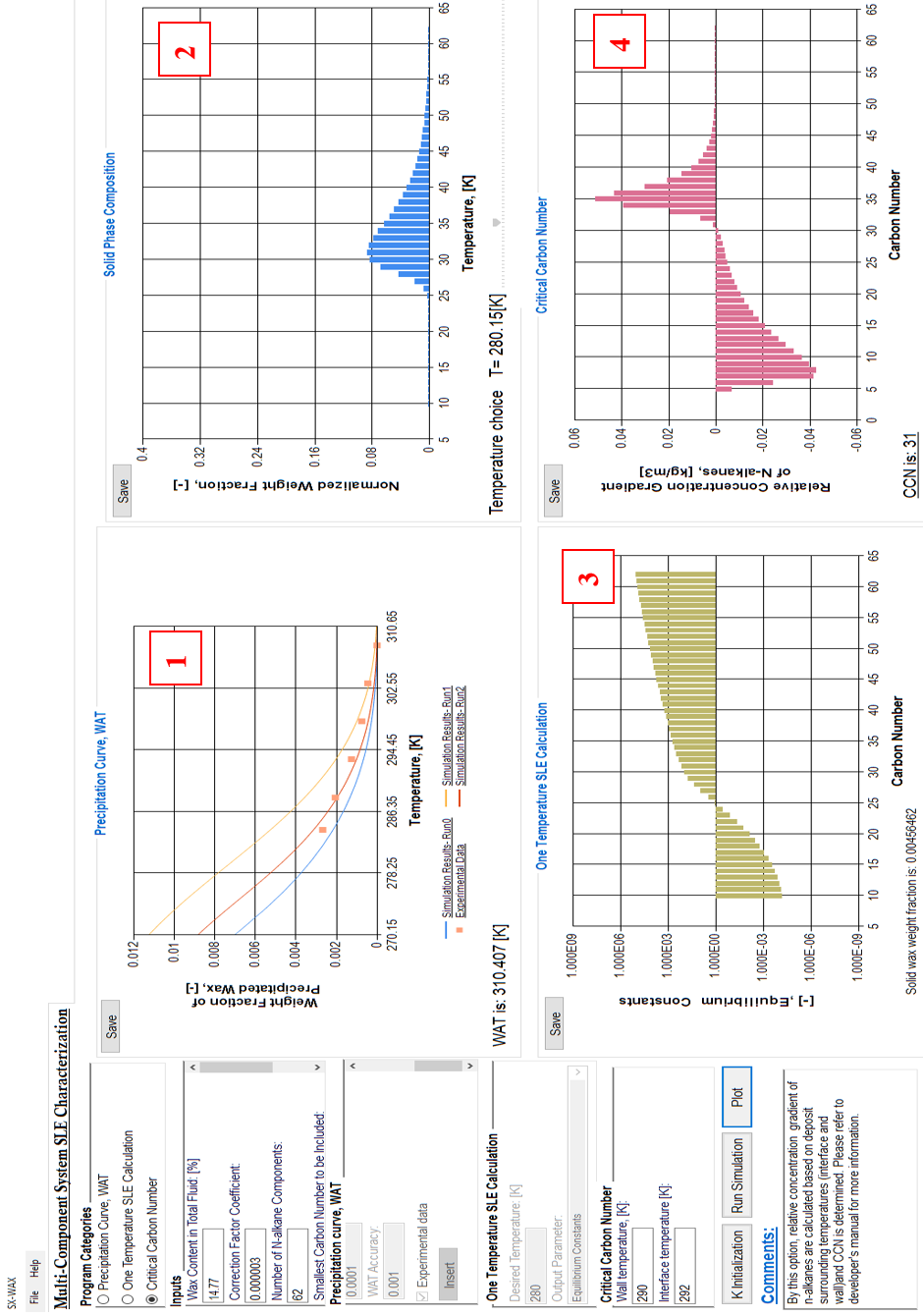


Figure 2: SP-Wax interface for multicomponent systems and its various functionalities. The inputs are given through different textboxes on the left of the screen and the plots are created. In 2.1predicted and experimental precipitation curves can be plotted, in 2.2solid-phase composition can be plotted for the given temperature range using a trackbar, in 2.3different SLE characteristics can be plotted (as desired) for the provided temperature point and, in 2.4relative 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 [38,39] were used for validating binary system prediction of SP-Wax. Data from these sources [38,39] 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, data from Panacharoensawad [10], Rittirong [31], Zheng et al. [34], and Fleming et al. [35] were used for the validation process. Oil types in Panacharoensawad [10], Rittirong [31], Zheng et al. [34], and Fleming et al. [35] are crude oil, crude oil, condensate, and pure paraffin mixture, respectively. Numerical values of the data are provided in “SP-Wax result.xlsx” excel file in the following directory https://github.com/epmmko/sp-wax

## 3.1 Binary System Validation

SP-Wax predictions have been validated with experimental data of five binary systems. The dissolved solute mole fractions at various WAT values from SP-Wax were compared with the literature data [38,39] 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.

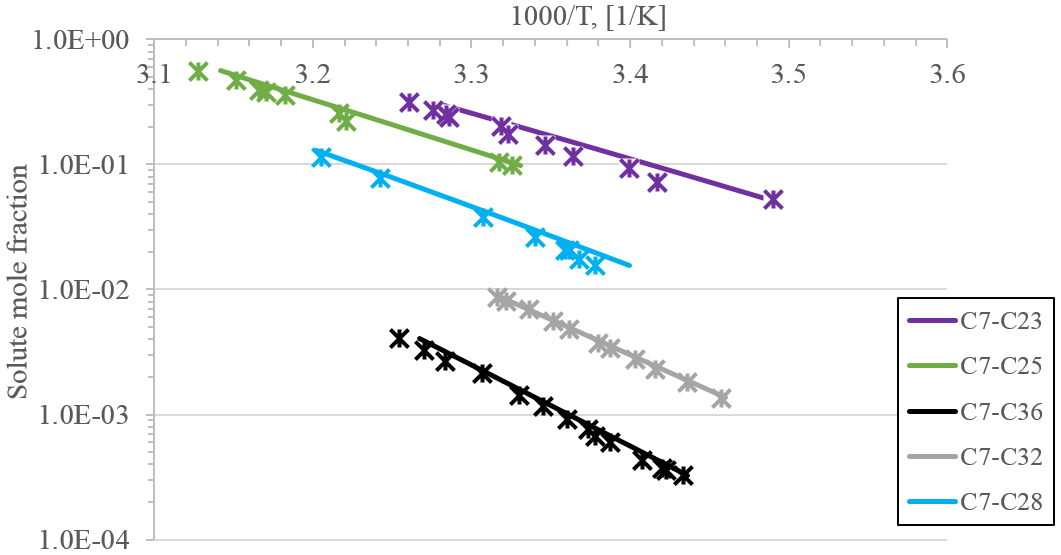


Figure 3: SP-Wax predictions and experimental data [38,39] ( symbol) of solid solubilities for five binary system at 1 bar

## 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 of Fleming et al. [35], Rittirong [31], and Zheng et al.’s [34] were used to validate SP-Wax software. Fleming et al. reported experimental and predicted precipitation data points. Their prediction was based on Coutinho et al.’s model [15] using UNIQUAC approach for solid-phase non ideality. For another case, Rittirong [31] reported experimental precipitation data along with simulation results of TUWAX and PVTsim thermodynamic software. Notably, SP-Wax is far more accurate than all other simulation results. Zheng et al.’s [34] 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 [13]. Zheng et al.’s [34] input composition for n-alkanes were reported graphically from C15 to C36. In our study, we extrapolated the composition for wider range of carbon numbers and made the prediction. The extrapolation is somewhat subjective and it is not unique. SP-Wax predictions of precipitation curve are in very good agreement with all three 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 this case. This is another indication of the validity of our developed thermodynamic software.

For Fleming et al. [35], 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. [34] and Rittirong [31], the optimum adjustment coefficient was chosen to be with of 0.95 and 0.96, respectively.

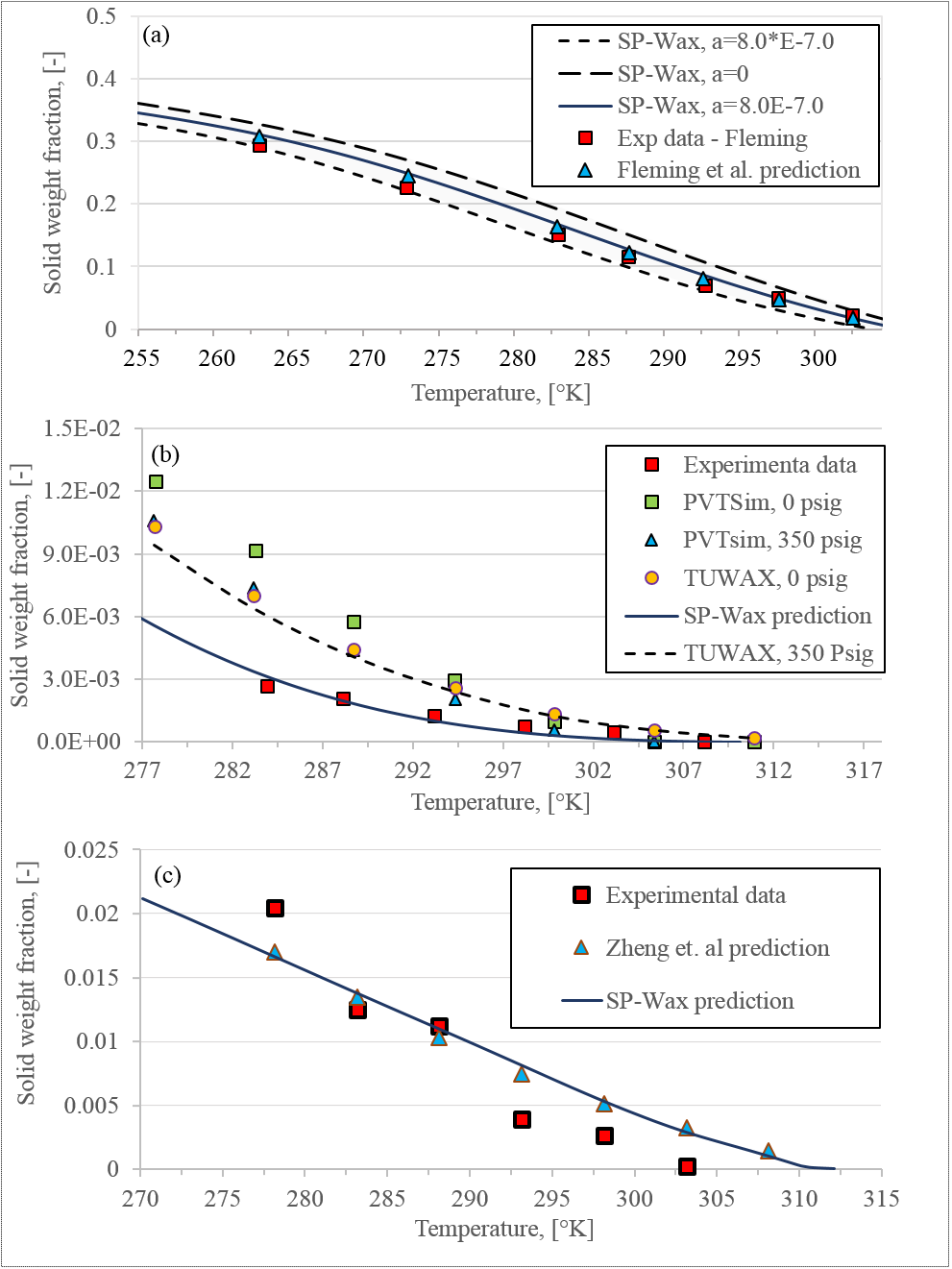


Figure 4: SP-Wax precipitation curve validation against Fleming et al.(a) [35], Rittirong(b) [31], and Zheng et al.(c) [34].

In addition to the precipitation curve prediction that is used in the pseudo-single-wax-phase modeling approach [4,11,10,31], solid phase composition information is also important for a compositional-based model [34] and for analyzing the CCN of wax deposit for both single-phase [3] and multiphase cases [1,14]. SP-Wax was validated through five sets of experimental CND data from Rittirong [31] and Panacharoensawad’s [10] single phase wax deposition test results. Figure 5 shows SP-Wax predictions against experimental solid-phase CND data. SP-Wax predictions are in good agreement with experimental data for all cases.

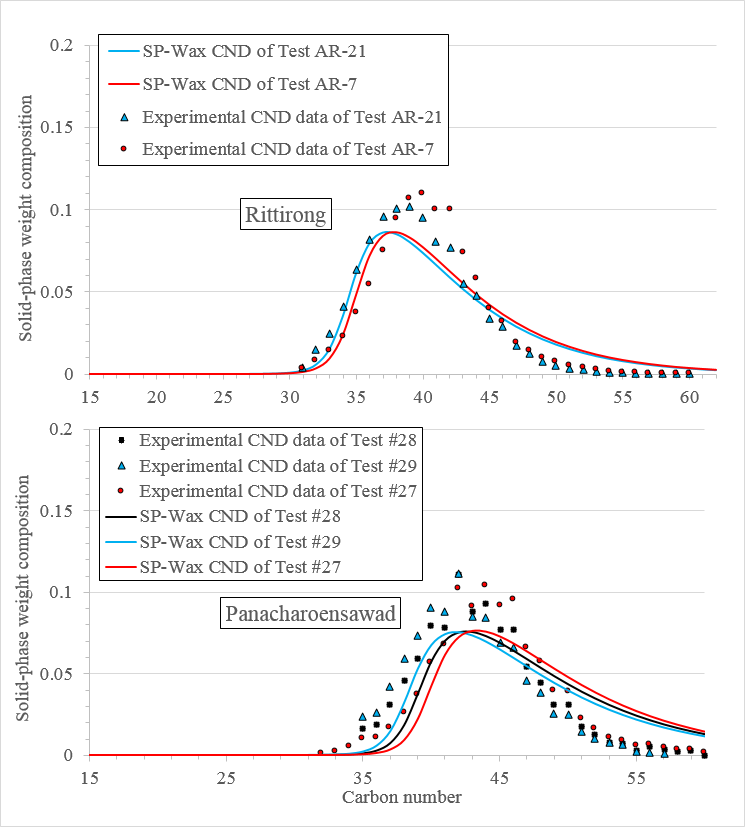


Figure 5: Solid-phase CND of paraffin deposit. SP-Wax predictions versus CND experimental data of Ritirrong [31] and Panacharoensawad [10] at average deposit temperature at the end of each test

The used temperatures for SP-Wax simulation are listed in Table 1. The slight overestimation from SP-Wax’s prediction is expected because, SP-Wax take only the final-time temperature and this temperature is always higher than the average temperature over the time of experiment.

Lastly, the CCN prediction from SP-Wax against the deposit data are shown here. This is not a direct model verification, but rather a model extension. This is because CCN prediction requires information of the deposit temperature at the flowing condition. SP-Wax uses the pre-calculated deposit value reported in the literature [10,31] and uses the relative concentration gradient to estimate CCN. The relative concentration gradient here is defined as the ratio of ith carbon number dissolved mass over the volume of n-alkanes in liquid phase (in m3). SP-Wax estimated CCN by using the smallest carbon number with positive relative concentration gradient from the carbon number versus the relative concentration gradient plot (Figure 6). We note that CCN determination typically requires significant overhead calculation as part of wax deposition modeling. However, this thermodynamic property (CCN) can be estimated as a function of deposit temperature. Since deposit’s temperature can be determined using experimental measurements, it can be used to predict CCN by SP-Wax

SP-Wax can roughly estimate the CCN with only information of the deposit temperature at the final time (the time at which the composition was determined by HTGC).

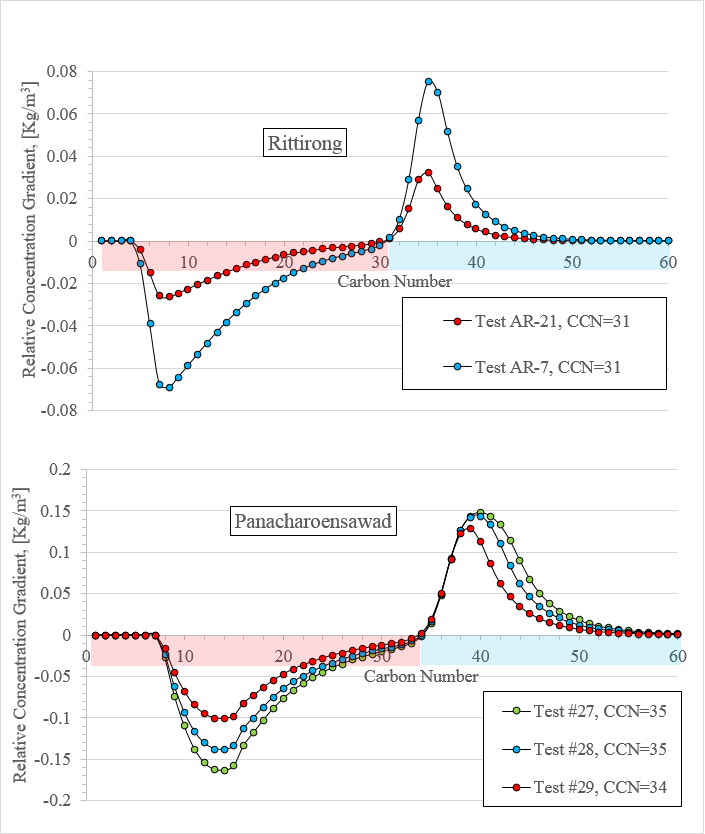


Figure 6: SP-Wax relative concentration gradient predictions for five tests of Ritirrong [31] and Panacharoensawad [10]. Associated CCN values are annotated in the graph for each test. Blue and red highlighted sections are referred to carbon number components that diffuse in and out of deposit, respectively.

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 of inner wall, deposit interface, and bulk fluid at the end of experiments for five tests plus experimental data [10,31] 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 [10] and Ritirrong [31], 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 absolute relative percentage error % is defined as .

The percentage relative error of the model prediction is shown in Table 2. This relative error is estimated from

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

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

Although, SP-Wax calculations are done in SI units (), the relative errors for solid solubility temperature (WAT) predictions in the binary systems are based on the Celsius degree (). This way of error calculation is more realistic although it results in higher magnitude of error. The detailed calculation and the numerical values of the data and prediction are shown externally in the supporting information section (<https://bit.ly/2zQYt7r>). Table 2 shows that the model have the average estimated relative error about 22% and 3.7% for the case of multicomponent precipitation curve and the binary system WAT, respectively. SP-Wax requires the accurate input n-alkane compositions. Multicomponent system tends to have a higher uncertainty than the binary system. Multicomponent system has a higher accumulative error of the input compositions than that of the binary system, because it simply has more components. In some multicomponent cases, such as in Zheng et al. [34] data, 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 solid solubilities of binary systems (Figure 3) and 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 |
| C7-C23 | Binary | 7.0 |
| C7-C25 | Binary | 2.9 |
| C7-C28 | Binary | 4.6 |
| C7-C32 | Binary | 1.0 |
| C7-C36 | Binary | 3.0 |

# Impact and Conclusions

The currently available thermodynamics software in the literature is either not open-source [41], or is open-source but does not have the SLE calculation for n-alkanes [42]. The problems with the undisclosed source code are 1) the code is not fully described, and it cannot be reviewed for potential bugs and errors 2) any further development requires the repetition of the coding efforts which has previously done. SP-Wax is the first open-source thermodynamic software for modeling various SLE characteristics of paraffin in binary and multicomponent systems. SP-Wax is one of the very few studies that compared thermodynamic model predictions to experimental solid phase composition data. 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 [15–22] and other literature [10,23–40] were coded in C++ with a user-friendly C# interface. Such C++/C# communication provides an excellent tool for technical and non-technical users to use the software. SP-Wax can be adopted by researchers with various areas of interest. Therefore, SP-Wax is, equipped with OpenMP parallel programming technique, and it is free of any convergence problems. 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. These data sets are five sets of solid phase composition of wax deposit, three precipitation curves, and CCN values of five cases. The comparison shows that SP-Wax successfully predicted these parameters. The comparison with experimental data showed that SP-Wax has the mean absolute average relative error of 22% for precipitation curve prediction and average relative error of for binary solid solubility cases. Furthermore, the mean absolute relative error from SP-Wax was found to be 5.5% for ACN and 1.9% for CCN predictions.

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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 or mole of solid / mole of total solution, [-]

Universal gas constant,

Parameter that is defined differently by different liquid-phase activity coefficient models

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

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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* |