# SP-Wax: Fully optimized SLE thermodynamic modeling software for paraffin

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# Abstract

The open-source software (SP-Wax) for solid-liquid equilibrium (SLE) calculation of paraffin is presented in this study. 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 developed software is based on Coutinho et al. models, and has been validated by binary and multi-component system data. 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. C# Windows Forms user interface was created to ensure the reusability of the software for both technical and non-technical users.

# Motivation and Significance

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), 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 in the pipe. Therefore, 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 study provides an open-source thermodynamics package with a user-friendly interface to promote the advancement of 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, too. This is because the thermodynamics of wax is very important for the deposition calculation in a complex multiphase flow.

# Software description

In this section, theoretical framework of the software is presented. SP-Wax is based on thermodynamic models of Coutinho and co-workers [15–22] and other literatures and other literatures [10,23–41]. In SP-Wax, the governing equations [36] are solved for non-ideal paraffinic solutions. The governing equations are:

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

The solid weight fraction was calculated from [30]:

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

Once the equilibrium constants, , and the solid mole fraction, , were determined, 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 Entropic free-volume model to express activity coefficient of liquid phase as [18]:

|  |  |
| --- | --- |
|  | (6) |
|  | (7) |
|  | (8) |

Molar volume ) is calculated through DIPPR correlations [28] for . For the rest of carbon number components ( or ), GCVOL group contribution method [41] was used. Van der Waals volumes ) for different carbon number components were calculated from Bondi et al. [29].

The solid phase activity coefficient of each component, , is needed for calculation in Eq. (1). However, researchers have difficulties to accurately quantifying the non-ideal behavior of the solid-phase. Coutinho et al. [17,20] suggested two different approaches including UNIQUAC and Wilson models. Wilson model is less computationally intensive compared to UNIQUAC model. It also gives accurate results. Therefore, Wilson model [17] is selected for calculating the solid-phase activity coefficients in SP- Wax. Wilson model is as follows:

|  |  |
| --- | --- |
|  | (9) |
|  | (10) | |
|  | (11) | |
|  | (12) | |
|  | (13) | |

Enthalpies of fusion and solid-phase transition () were calculated using correlations proposed by Coutinho et al. [19]. Extension of Pitzer CSP model [25] was used to calculate enthalpies of vaporization ().

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 shorts 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, 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 literatures. Coutinho et al. [21] introduced a correlation for correction factor in binary systems. Yang et al. [24] suggested using Coutinho’s correlation [21] in multi-component systems for components with similar sizes and proposed a new relation for components with different sizes. A new approach for calculating correction factor was proposed by Coutinho et al. [20] which related enthalpies of sublimation () to In their paper [20], several multi-component paraffinic systems were successfully analyzed using the proposed correction factor. In SP-Wax, an adjustable coefficient was used instead of a constant value of used in Coutinho et al. [20] (shown below) was used. This worked well for all multi-component systems.

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

It is advised to manually adjust the value of to match the precipitation curve if experimental data points are available. However, if there is no experimental data, we suggest following values for .

|  |  |
| --- | --- |
|  | (16) |
|  | (17) |
|  | (18) |

We compared experimental data of four multi-component 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 (), 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.[35]. This additional analysis is to show that SP-Wax can estimate the deposit composition (specially 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 [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 [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.

* 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 calculate the solid and liquid phase compositions of the system by solving 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 value 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 multi-component 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 software’s prediction. In multi-component 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 intensively in wax deposition simulations [4,11,31,42,43]. 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 multi-component system is to calculate and report various SLE properties of the system at one desired temperature (SPWaxOneTemperatureCase.cpp). By this program option, 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 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 sample 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 multi-component simulation option enables the user to plot relative concentration gradients of all carbon numbers. In this graph, smallest carbon number with positive relative concentration gradient is Critical Carbon Number and it is reported by SP-Wax. Please refer to developer’s manual for more information about required inputs and program options. The following picture shows SP-Wax software interface for multi-component systems.

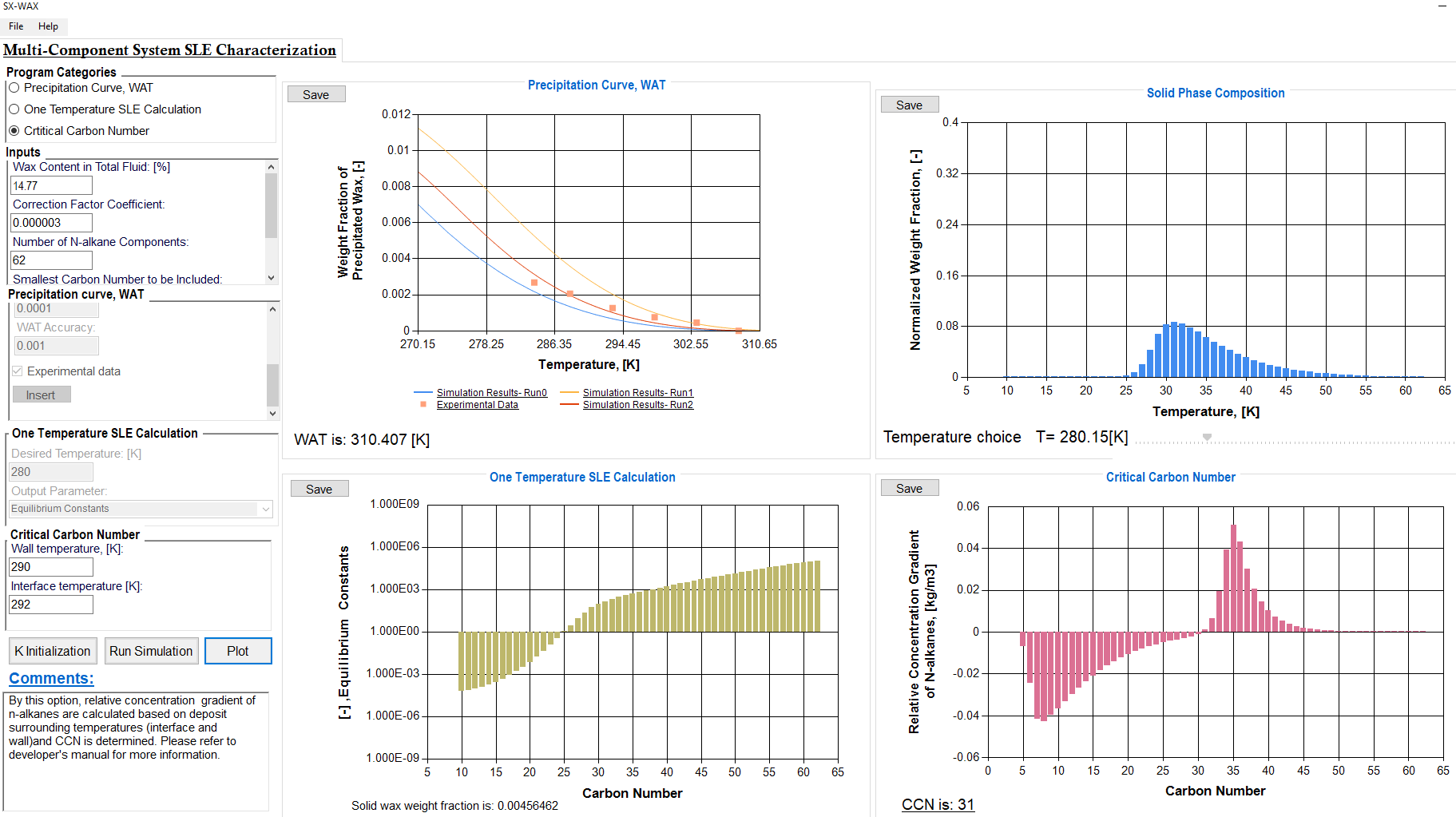


Figure 2: SP-Wax interface for multi-component systems and its various functionalities.

# 3.0 Illustrative Examples

*3.1 Binary System Validation*

SP-Wax predictions have been successfully validated with experimental data of five binary systems. The dissolved solute mole fraction at various WAT values from SP-Wax was compared with the literature data [38,39]. 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: Predictions and experimental data ( symbol) of solid solubilities for five binary system at 1 barwith values (square of the Pearson product moment correlation coefficient)

*3.2 Multi-component System Validation*

Fleming et al.[37], Rittirong[31], and Zheng et al.[35] precipitation data were used to validate SP-Wax precipitation prediction. Fleming et al. reported experimental precipitation data points (from micro-Differential Scanning Calorimetry) and prediction of precipitation curve using Coutinho et al. model [15]. Rittirong [31] results are DSC-based precipitation data. Zheng et al. [35] 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]. 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. prediction, even though Fleming et al. used UNIQUAC model for the solid-phase non-ideality.

For Fleming et al.[37], precipitation curves with three different values of adjustment parameter were calculated and shown. In their case, only n-alkane components were present () and very small adjustment was needed. Among the three curves, the best fit was resulted from with . For oil cases of Zheng et al.[35] 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.[37] result (a), and Zheng et al.[35] and Rittirong [31] (b).

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 [35] 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 [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

In Figure 5, deposit temperature used for SP-Wax calculation is the average of the wall temperature that the deposit was in contact with and the deposit-oil interface temperature () at the end of each test. The temperatures used for SP-Wax simulation are listed in Table 1.

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 use 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, SP-Wax can roughly estimate the CCN with just 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 graphical form above, 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, Critical Carbon Number (CCN). South Pelto and Garden Banks are the names of oil sample 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 .

In Table 2, coefficient of determination () for binary solid solubilities and multi-component precipitation curves are provided. Resulted values are very close to 1.0 which is another indication of SP-Wax accuracy.

Table 2: Comparison of SP-Wax prediction and experimental data, using coefficient of determination (r2) for solid solubilities of binary systems and precipitation curves of multi-component systems. r2 is the square of the Pearson product moment correlation coefficient.

|  |  |  |
| --- | --- | --- |
| Case | System | R2 |
| **Rittirong** | Multi component | 0.96 |
| **Zheng et al.** | Multi component | 0.95 |
| **Fleming et al.** | Multi component | 0.997 |
| **C7-C23** | Binary | 0.982 |
| **C7-C25** | Binary | 0.996 |
| **C7-C28** | Binary | 0.998 |
| **C7-C32** | Binary | 0.999 |
| **C7-C36** | Binary | 0.998 |

# Impact and Conclusions

Despite the recent efforts, engineering open-source software [44–46] is still limited. The currently available thermodynamics software in the literature is either not open-source [47], or open-source but does not have the SLE calculation for n-alkane[48]. This software will directly benefit various researchers and industries that need the SLE calculation of paraffinic wax, 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. SP-Wax is the first open-source thermodynamic software for modeling various SLE characteristics of paraffin in binary and multi-component systems.

SLE thermodynamic model from Coutinho and co-workers [15–22] and other literatures [10,23–41] 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 fully-optimized, equipped with OpenMP parallel programming technique, and it is free of any convergence problem. SP-Wax comes with complete user and 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 multi-component 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 minimum r-squared value of 0.95 for precipitation curve prediction and the minimum of for binary solid solubility cases. The mean absolute relative error from SP-Wax was found to be 5.5% for ACN and 1.9% for CCN prediction.

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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,

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, [-]

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, [-]

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 Waal

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)* |
| S4 | Computing platform / Operating System | *Microsoft Windows* |
| S5 | Installation requirements & dependencies | *Microsoft Windows operating system* |
| S6 | If available Link to user manual - if formally published include a reference to the publication in the reference list | *https://github.com/epmmko/sp-wax/Manuals* |
| S6 | Support email for questions | [*ekarit.panacharoensawad@ttu.edu*](mailto:ekarit.panacharoensawad@ttu.edu)  *arya.shahdi@ttu.edu* |