Modeling Displacement Efficiency Improvement During Solvent Aided-SAGD
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Abstract
Coinjection of small amounts of hydrocarbon solvents with steam has the potential to improve the oil recovery efficiency while reducing the energy intensity of conventional SAGD (steam assisted gravity drainage). A number of studies have reported lower residual oil saturations inside the coinjection chamber compared to SAGD. There is, however, no mathematical model available to predict the extent of such displacement efficiency improvement or to compare it during the coinjection of different solvents.

This paper presents a mathematical procedure for the estimation of local displacement efficiency improvement in the coinjection process. Displacement efficiency is modeled as a function of local solvent accumulation, upon the arrival of coinjection chamber interface, and the temperature, as the region is swept by the chamber. The model is used to investigate the interaction of displacement efficiency improvement, ultimate bitumen recovery, and solvent retention inside the swept region, the last of which is of significant concern in large scale applications.

The complex interaction of mass and energy flow is simplified without loss of the fundamental mechanisms and phase behavior details. Initially, phase equilibrium equations are solved to find the thermodynamic conditions inside and at the boundary of the coinjection chamber. Then, the saturation of phases as well as the retained amount of solvent are estimated along the temperature profile inside the chamber by making reasonable assumptions. The model is also used to investigate the impact of changing a solvent-steam coinjection ratio on the displacement efficiency improvement and/or solvent retention.

Results indicate that coinjection can achieve improved displacement efficiency even without modifying the end point saturations of the relative permeability curves as a result of solvent coinjection. Eventually, the results are validated by using numerical simulations for the coinjection process. It is demonstrated that a robust understanding of phase behavior interaction with heat and solvent transport is critical to explaining the recovery mechanisms involved in solvent-aided SAGD.

Introduction
The main challenge in the recovery of oil from oil sands is the extremely high viscosity which renders the oil essentially immobile at initial reservoir conditions. SAGD is a widely used in situ recovery technique to extract bitumen from Alberta’s oil sands (Butler 1997). SAGD uses a pair of horizontal wells that are drilled on the top of each other with an inter well spacing of a few meters. High quality steam is injected through the upper horizontal well and propagates into the reservoir in the form of a steam chamber. Steam, in contact with cold bitumen, releases its latent heat and mobilizes the bitumen. The mobilized bitumen along with the condensed water drain towards the producer under the effect of gravity, where they can be transported to surface.

SAGD is an energy intensive process with some economic and environmental concerns. Coinjection of small amounts of solvent with steam has emerged as one of the alternative recovery techniques to improve the efficiency of SAGD. The idea is to take advantage of both heat transfer from steam and diluting effects from solvents to mobilize the bitumen at lower temperatures and thus reduce the energy intensity of the process.

Steam and solvent coinjection has been implemented in lab, pilot and field scales under various commercial names. Typical solvents selected for coinjection include pure hydrocarbons ranging from C$_3$ to C$_{12}$ and diluents. Heavier solvents (C$_{16}$ to C$_{20}$) were also tested but did not improve the recovery (Shu and Hartman 1988). Successful applications of coinjection have reported improved oil production rates and reduced steam-oil ratios (SOR) compared to steam-only injection (Nasr et al.
A number of numerical, analytical and laboratory studies have investigated the effects of solvent type, solvent-steam co-injection ratio and co-injection strategy on the oil production rate (Nasr et al. 2003; Gupta and Gitting 2007b; Gupta and Gittins 2012; Jha et al. 2013; Keshavarz et al. 2014b; Li et al. 2011b; Shu and Hartman 1988; Yazdani et al. 2011; Rabiei et al. 2014). The results, however, are not always consistent with each other as described by Keshavarz et al. (2014b). Keshavarz et al. (2014bc) conducted numerical and semi-analytical studies of co-injection with a SAGD well pattern. They showed that the choice for optimum solvent and co-injection strategy is impacted by the operating conditions as well as bitumen’s viscosity-temperature behavior.

A few studies have also indicated that co-injection of solvent with steam has the potential to reduce the residual oil saturation below that of a steam-only injection process. Nasr and Ayodele (2006) studied the co-injection of a mixture of C₄-C₁₀ with steam in experiments with a Cold Lake type of bitumen. They observed lower residual oil saturations in their co-injection experiments compared SAGD. Li et al. (2011a) conducted solvent-aided-SAGD experiments with the Athabasca bitumen and two different solvents: C₇ and a mixture of C₇ and xylene. They reported that the ultimate recovery factor inside the experimental cell was improved from 25% after pure steam injection to 29% and 34% when C₇ and a mixture of C₇ and xylene were co-injected with steam, respectively. Yazdani et al. (2011) also reported lower residual oil saturations in their numerical simulations of co-injection compared to SAGD. They attributed this improved displacement efficiency to the interfacial tension (IFT) reduction between phases during steam-solvent co-injection and the solvent amount in the residual oil phase. Hosseininejad Mohebati et al. (2012) conducted laboratory experiments of SAGD and hexane co-injection with steam during SAGD. Comparison of their post-test sand samples showed a considerably lower residual oil saturation inside the sample under co-injection compared to SAGD (residual oil saturations as low as 0.4% were observed in the post-co-injection test sand sample).

As mentioned by Jha et al. (2013), there were attempts in the literature to model the lower residual oil saturation inside a co-injection chamber by modifying the saturation end points of the relative permeability curves. These included using small residual oil saturations to gas (Gates 2007; Ardali et al. 2011) or using composition dependent residual saturations (Ivory et al. 2010). These modifications, however, still need further investigations.

Jha et al. (2013) and Keshavarz et al. (2014a) conducted numerical simulations on steam and solvent co-injection with a SAGD well pair. They demonstrated that the lower residual oil saturation inside a co-injection chamber, compared to SAGD, can be achieved without modifying the end point saturations of relative permeability curves. They explained the potential for displacement efficiency improvement during co-injection as a result of the interaction of solvent accumulation, temperature variation and phase equilibrium in the co-injection simulations.

Keshavarz et al. (2014a) demonstrated that there are two key mechanisms that contribute to the improved displacement efficiency during a co-injection process: 1) accumulation of solvent near the chamber interface which lowers the bitumen concentration there and 2) redistribution of the diluted oil with solvent in the gaseous and oleic phases in the presence of the water phase during further chamber propagation. Keshavarz et al. (2014b) showed how a co-injection strategy can be designed to maximize the displacement efficiency improvement resulting from the above mechanisms.

The above explanation for displacement efficiency improvement during co-injection is consistent with experimental results of Nasr and Ayodele (2006) and Hosseininejad Mohebati et al. (2012). Regions with improved displacement efficiency in the experiments of Hosseininejad Mohebati et al. (2012) correspond to regions that have experienced a high solvent accumulation during propagation of the co-injection chamber (i.e., the first mechanism described above). Also, a low solvent concentration was observed in the regions with lowered residual oil saturation in the experiments conducted by Nasr and Ayodele (2006), which is an indication of solvent re-evaporation from these regions (i.e., the second mechanism described above).

In addition to a limited number of experimental and numerical studies, there is no mathematical procedure available in the literature to model the displacement efficiency improvement during co-injection. Thus, the main objective of this paper is to model the mechanisms of displacement efficiency improvement as described by Keshavarz et al. (2014a) mathematically.

Single component solvent-steam co-injection is studied with a SAGD well pattern and is referred to as solvent aided-SAGD (SA-SAGD) in this work. C₇ is selected as the single component solvent in this work. Phase equilibrium equations are initially solved for a ternary system of steam, solvent and bitumen inside and at the boundary of the chamber. Phase saturations inside the chamber are then estimated by making reasonable assumptions.

The model can be used to estimate the amounts of bitumen that is displaced from within the co-injection chamber as well as the amount of solvent which is retained inside the chamber. The model will be also utilized to demonstrate the impact of variation in the solvent steam co-injection ratio (SSR) on displacement efficiency improvement and solvent retention. The improved knowledge obtained from the model can be utilized to design a co-injection strategy that minimizes the residual oil saturation and/or solvent retention inside the co-injection chamber.

Predictions form the model will be validated by fine scale numerical simulations. The impact of solvent type and operating pressure are other important parameters which will remain as the subject of a future study.
Phase Equilibrium Conditions Inside and at the Boundary of the Coinjection Chamber

In this section, a calculation procedure is presented for estimating the thermodynamic conditions inside and at the edge of a SA-SAGD chamber. Results of phase equilibrium calculations will be used in the subsequent section of this paper to estimate phase saturations inside the coinjection chamber. The following simplifying assumptions are made with respect to calculations in this section: (1) ternary mixtures of water, single-component solvent and single-component oil, (2) complete immiscibility between the oleic (L) and aqueous (W) phases, (3) constant pressure inside the chamber, and (4) Raoult’s law for phase equilibrium.

Inside the SA-SAGD chamber three equilibrium phases, L, W and V (V stands for the vapor phase), co-exist. Thus, the degree of freedom will be 2 according to Gibb’s phase rule. For a fixed operating pressure, a temperature and composition gradient can exist inside a coinjection chamber. A chamber edge in this study is defined where the transition from L-W-V equilibrium to L-W equilibrium occurs. For a fixed overall composition, the chamber edge temperature ($T_{edge}$) is the lowest temperature at which the system can accommodate the V phase.

Figure 1 taken from Keshavarz et al. (2014c) illustrates the conditions inside and at the interface of the coinjection chamber for an assumed pressure and temperature. Note that the W phase consists of 100% water, and the L phase does not contain the water component. $T_{edge}$ is the same for any overall composition on the L-W edge of the tie triangle.

For a given operating pressure, composition of the equilibrium phases can be uniquely determined once the temperature is fixed. Figure 2 shows the results of these calculations for ternary mixtures of water, bitumen and C₃, assuming Raoults law for phase equilibrium. The corresponding equations are presented in Appendix 1. An operating pressure of 2,000 kPa is assumed in calculations. Typical properties for Athabasca bitumen (GCOS) are taken from Mehrrota and Srvcsek (1987) and presented in Table 1 along with the properties of water and solvent.

Temperature will gradually drop from the point of injection towards the coinjection chamber interface and solvent concentration will start to build up in both the V and L phases according to Figure 2. The maximum temperature in the coinjection chamber ($T_{max}$) occurs at the point of injection and is a function of the solvent-steam coinjection ratio on a molar basis (SSR) through the following equation:

$$x_w = \frac{p_{w}(T)}{p}$$

where $x_w$ and $p_{w}(T)$ are the mole fraction of water in the V phase and the saturation pressure of water as a function of temperature at the point of injection, respectively. For a prescribed SSR and operating pressure, the above equation can be solved for $T = T_{max}$. Note that $T_{edge}$ may vary between the two ends of the horizontal axis in Figure 2, depending on solvent accumulation at the chamber edge. The minimum possible $T_{edge}$ occurs where the local mixture is composed of water and solvent component only (i.e., solvent mole fraction in the L phase ($x_{SL}$) = 1.0). This is the temperature estimated by Dong (2012) as the three phase temperature of water-solvent binary.

Estimation of Phase Saturations inside the chamber

This section extends the phase equilibrium calculations to estimate the saturation of phases inside and at the interface of the SA-SAGD chamber. The following assumptions are made in addition to assumptions of the previous section: (1) a step-change in the L phase saturation at the chamber interface from its value outside the chamber to the residual L phase saturation of the gas liquid system ($S_{L}$), (2) dead reservoir oil; i.e., concentration of the reservoir oil component in the V phase is negligible, and (3) temperature and composition-independent residual L and W phases’ saturations that are identical for SAGD and all SA-SAGD cases.

Consider a sufficiently small control volume (CV) of the reservoir to which uniform rock and fluid properties can be assigned. The calculation procedure involves tracking of equilibrium phases’ compositions and saturations of this CV upon the arrival of the chamber edge and afterwards. Saturation of the L phase can be related to its composition through the following equation:

$$S_L = \frac{N_{IL}}{x_{IL} \rho_L}$$

where $S_L$ and $\rho_L$ are the saturation and the molar density of the L phase, respectively, $x_{IL}$ is the mole fraction of component i ($i =$ solvent (s) or bitumen (b)) in the L phase, and $N_{IL}$ is the mole number of component i in the L phase per pore volume of the CV.

Values of $x_{IL}$, at the specified P and any T inside or at the boundary of the chamber are obtained from the results of phase equilibrium calculations in the previous section. $\rho_L$ is calculated using the following mixing rule:

$$\frac{1}{\rho_L} = \sum_i \frac{x_{IL}}{\rho_{IL}}$$
where \( \rho_{li} \) is the liquid density of component \( i \). Molar densities of solvent and bitumen components as a function of pressure and temperature are estimated using the following correlation in this work:

\[
\rho_l = \rho_l^0 \cdot \exp(\alpha_c (P - P_{ref}) - \alpha_1 (T - T_{ref}) - 0.5\alpha_2(T^2 - T_{ref}^2))
\] ..........................(4)

where \( P_{ref} \) is the reference pressure, \( T_{ref} \) is the reference temperature, and \( \rho_l^0 \) is the reference molar density of component \( i \) as reported in Table 2. \( P_{ref} \) and \( T_{ref} \) are taken as 101.3 kPa and 15°C, respectively. \( \alpha_c, \alpha_1, \) and \( \alpha_2 \) are compressibility, and first and second thermal expansion coefficients, respectively, and listed in Table 2.

For a specified operating pressure and an assumed solvent molar concentration of the \( L \) phase at the chamber edge (\( X_{L,edge}^i \)), \( T_{edge} \) can be estimated using phase equilibrium calculations. Then for a given \( S_{L,edge} \) at the chamber edge (recall assumption (1) in this section), Equation (2) can be rearranged to obtain the mole numbers of bitumen (\( N_{s,L} \)) and solvent (\( N_{s,L} \)) components in the \( L \) phase per pore volume of the CV at the chamber edge.

As the chamber propagates further, the temperature of the CV will increase. The solvent portion of the \( L \) phase will be partially evaporated. This, in turn, will result in a reduction in the \( L \) phase saturation as discussed by Keshavarz et al. (2014a). Note that the reduction in \( S_L \) to values below \( S_{L,edge} \) is only due to redistribution of solvent component between \( L \) and \( V \) phases. The amount of the bitumen component in the \( L \) phase remains unchanged due to assumptions (2) and (3). Thus, keeping \( N_{s,L} \) constant, Equation (2) can be directly used to calculate \( S_L \) at \( T > T_{edge} \) (i.e., conditions inside the coinjection chamber) for \( i = o \). Due to assumption (3), this calculation does not account for the possible changes in temperature and/or \( L \) phase composition on the saturation end points of relative permeability curves. Having \( S_L \) for any \( T > T_{edge} \), the amount of solvent retention in the \( L \) phase per pore volume of the CV can be estimated by Equation (2) for \( i = s \). Saturation of the \( V \) phase for the CV inside the chamber can be calculated using:

\[
\sum_j S_j = 1.0 \quad (j = W, L \text{ and } V),
\] ..........................(5)

where \( S_j \) is the saturation of phase \( j \) in the CV. Assuming the \( W \) phase saturation (\( S_w \)) to be equal to the irreducible water saturation (\( S_{w,irr} \)) inside the chamber, the above equation can be solved for the unknown \( V \) phase saturation (\( S_v \)). Water saturation may be slightly higher than \( S_{w,irr} \) for the swept regions close to the chamber edge due to partial condensation of steam; however, the difference will get insignificant as the chamber propagates further and the CV falls in deeper parts of the coinjection chamber.

To calculate the amount of solvent retention in the \( V \) phase inside the chamber, the molar density of the \( V \) phase is first calculated using:

\[
\rho_V = \frac{p}{zRT},
\] ..........................(6)

where \( \rho_V \) is the \( V \) phase molar density, \( R \) is the universal gas constant equal to 8.31446 in SI and \( z \) is the \( V \) phase compressibility factor. The \( V \) phase is assumed to behave as an ideal mixture and \( z \) may be assumed 1.0. As stated in Appendix 1, the accuracy of estimations will be improved if an equation of state is used for phase equilibrium calculations to capture the deviations from ideality. Once \( \rho_V \) is obtained, the mole numbers of solvent in the \( V \) phase per pore volume of CV (\( N_{s,V} \)) is calculated from:

\[
N_{s,V} = S_V \cdot \rho_V \cdot x_{s,V}
\] ..........................(7)

This, along with \( N_{s,L} \) calculated from Equation (2), provides an estimate of the solvent content of the CV as it is engulfed by the coinjection chamber. The whole calculation procedure described above is repeated for discrete values of \( X_{L,edge}^i \) along the entire mixing line of solvent and bitumen, and discrete values of \( T \) ranging from the corresponding \( T_{edge} \) to \( T_{sat} \). The accuracy of calculations increases as the mole fraction and temperature steps are taken smaller.

A more useful application of these calculations is to evaluate the average values, in turn, may be used to estimate the amounts of retained solvent and displaced bitumen within the swept region. For a given size of a SA-SAGD chamber, porosity and \( T_{edge} \) (which is a function of time but may be averaged.
during the period of chamber propagation:
\[ N_s = V_{ch} \cdot \phi \cdot \left( N_{Ls}^{avg} + N_{Sv}^{avg} \right) \] ..............................(9)
\[ Q_o = V_{ch} \cdot \phi \cdot (S_{Lr} - s_{av}^{avg} \cdot (1 - C_{sL}^{avg})) \] ..............................(10)
where \( V_{ch} \) is the volume of the chamber, \( \phi \) is the porosity, \( S_{Lr} \) is the initial oil saturation, \( N_s \) is the mole numbers of the retained solvent inside the chamber and \( Q_o \) is the cumulative volume of displaced bitumen from within the chamber. \( C_{sL}^{avg} \) is the volumetric concentration of solvent retained in the residual \( L \) phase at \( T_{ch}^{avg} \) obtained from:
\[ C_{sL}^{avg} = \frac{x_{sL}^{avg} \cdot \rho_s^{avg}}{x_{sL}^{avg} \cdot \rho_s^{avg} + x_{vL}^{avg} \cdot \rho_v^{avg}} \] ..............................(11)
where \( x_{sL}^{avg} \) and \( \rho_{sL}^{avg} \) are the mole fraction in the \( L \) phase and density of component \( i \) at \( T_{ch}^{avg} \). Note that the \( N_s \) calculated above is due to thermodynamic equilibrium inside the swept region and does not account for solvent trapping due to heterogeneities.

**Algorithm for Calculation**
The following steps are taken to obtain \( S_{Lr}^{avg}, N_{sL}^{avg} \) and \( N_{sv}^{avg} \) along the entire mixing line of solvent and bitumen at the chamber edge:

1. Solve the phase equilibrium equations (see Appendix 1) for ternary mixtures of water, solvent and bitumen at the specified operating pressure and temperatures ranging from \( T_{w, sat} \) to the three-phase temperature of the water-solvent binary.
2. For a given SSR, calculate \( T_{max} \), using Equation (1). Find the minimum possible solvent concentration in the \( L \) phase at the chamber edge (\( x_{sL}^{edge,min} \)) corresponding to \( T_{max} \) using the results of Step 1.
3. For \( x_{sL}^{edge,min} \leq x_{sL}^{edge} \leq 1.0 \), find:
   - The corresponding \( T_{sL}^{edge} \) from results of Step 1.
   - \( \rho_L \) at the chamber edge using Equations (3) and (4).
   - The corresponding \( N_{oL} \) at the chamber edge using Equation (2) for a given \( S_{Lr} \).
4. Find the average chamber temperature (\( T_{ch}^{avg} \) is estimated by Equation (8) in this work), the corresponding \( x_{sL}^{avg} \) from the results of Step 1, as well as \( \rho_{sL}^{avg} \) and \( \rho_{vL}^{avg} \), from Equations (3), (4) and (6).
5. Calculate \( S_{Lr}^{avg} \) and \( C_{sL}^{avg} \) using Equations (2) and (5) for a given \( S_{W/L} \).
6. Calculate \( N_{sL}^{avg} \) and \( N_{sv}^{avg} \) using Equations (2) and (7).

Steps 3 to 6 are repeated for different values of \( x_{sL}^{edge} \). The last two steps give the average saturations of the \( V \) and \( L \) phases as well as the average solvent retention in each phase per pore volume of the CV for the specified \( S_{sL}^{edge} \).

**Results and Discussion**

Figure 3 presents the results of sample calculations for coinjection of \( C_5 \) with steam at a pressure of 2,000 kPa. \( S_{Lr} \) and \( S_{W/L} \) are assumed to be 0.13 and 0.25, respectively. Other component properties are picked from Tables 1 and 2. The two horizontal axes represent the solvent concentration in the \( L \) phase when the CV is located at the chamber edge and the temperature of the CV after being engulfed by the chamber. Temperature and mole fraction steps are taken as 1.0 °C and 0.1, respectively. Phase properties at intermediate values of \( T \) and \( x_{sL}^{edge} \) are interpolated for plotting purposes.

Since \( T_{sL}^{edge} \) and \( x_{sL}^{edge} \) are interdependent, the temperature interval will span along the \( x_{sL}^{edge} \)-axis. According to Figure 3, for a fixed \( x_{sL}^{edge} \), \( S_{Lr} \) will reduce as temperature of CV increases. This simulates the continuous evaporation of the solvent for a specific CV as it is engulfed by the chamber and experiences higher temperatures in deeper parts of the chamber. This results in circulation of solvent in the vicinity of the chamber edge.

The two ends of the solvent-bitumen mixing line correspond to two limiting cases. A zero value for \( x_{sL}^{edge} \) at the left end corresponds to a SAGD type of process where no reduction of residual oil saturation below \( S_{Lr} \) will occur. A value of unity for \( x_{sL}^{edge} \) at the right end corresponds to the situation when the \( L \) phase at the chamber interface is composed of solvent component only. This can occur at certain stages of the coinjection process depending on the amount and duration of solvent coinjection and the removal rate of solvent from the chamber interface. Theoretically, such a condition will result in 100% displacement efficiency (i.e., a zero residual oil saturation) as soon as the corresponding CV is engulfed by the coinjection chamber and its corresponding temperature increases.

According to this analysis and as mentioned by Keshavarz et al. (2012), displacement efficiency improvement is considerable for regions that have experienced: (1) a sufficiently high solvent accumulation upon the arrival of chamber edge.
and (2) a sufficient temperature increment as the chamber propagates further and engulfs those regions. The absence or inefficiency of either of these two requirements impairs the displacement efficiency improvement.

It should be noted that the ultimate recovery factor of bitumen is only a function of $x_{sl}^{edge}$. Increasing $x_{sl}^{edge}$ is equivalent to replacing the residual bitumen with solvent at the chamber edge. Then, the second requirement for displacement efficiency improvement contributes to solvent recovery, but not to the bitumen recovery under the assumptions of this study. Figure 4 presents the mole numbers of solvent retained in the L and V phases per pore volume of CV as a function of $T$ and $x_{sl}^{edge}$. For a fixed $x_{sl}^{edge}$, the amount of solvent retention in both the L and V phases reduces as the temperature of CV increases. This means that the accumulated solvent will gradually leave the CV towards the colder regions, as it is engulfed by the chamber and its corresponding temperature increases.

Figure 5 presents the curves of $S_{br}^{avg} \cdot N_{sl}^{avg}$ vs. $x_{sl}^{edge}$. A solvent concentration of 4.0 mol% in the injectant is selected in the calculation of $T_{ch}^{avg}$ resulting in a $T_{max}$ of 210.3°C and $x_{sl}^{edge,min}$ of 2 mol%. According to Figure 5, the residual L phase saturation is a decreasing function of $x_{sl}^{edge}$. The slope of this decrease will be considerably sharper for $x_{sl}^{edge} > 0.7$. The amount of solvent retention in the L phase (per pore volume of CV) is not a monotonic function of $x_{sl}^{edge}$. For values of $x_{sl}^{edge}$ increasing from 0.0 to 0.7, solvent retention in the L phase also increases. This is due to the fact that the displacement efficiency improvement cannot compensate the incremental amount of solvent accumulation for $x_{sl}^{edge}$ values below 0.7. For values above this, however, the displacement efficiency will be improved with a much sharper slope; i.e., the reduction in the residual L phase saturation is as significant, even for a small increment in $x_{sl}^{edge}$, as the overall effect is a reduction in solvent retention in the L phase. The amount of solvent retention in the V phase (per pore volume of CV) is an increasing function of $x_{sl}^{edge}$.

Effect of Solvent-Steam Coinjection Ratio (SSR)

SSR will affect the mechanics of the process by altering the coinjection temperature, the average chamber temperature and the average value of $x_{sl}^{edge}$ during the process. Figure 6 shows the profiles of the residual L phase saturation and the retained amounts of solvent in the L and V phases at $T_{ch}^{avg}$ when the solvent mole fraction in the injectant is increased to 0.16. This will result in a coinjection temperature of 203.7°C at an operating pressure of 2.000 kPa. Thus, the maximum temperature at the chamber edge will be 203.7°C which corresponds to a $x_{sl}^{edge,min}$ of 0.09 according to Figure 2.

Comparison of Figure 6 with Figure 2 indicates that increasing the SSR from 0.04 to 0.16 will increase the average residual L phase saturation and solvent retention in both the L and V phases inside the chamber for a fixed $x_{sl}^{edge}$ ($x_{sl}^{edge} \geq 0.09$). It should, however, be noted that using a higher SSR will expedite the accumulation of solvent at the chamber edge; i.e., a higher average $x_{sl}^{edge}$ may be expected during the process. This, in turn, will enhance and expedite the displacement efficiency improvement (i.e., local displacement efficiency improvement will be observed in regions closer to the well pair). The above knowledge can also be utilized in designing a coinjection procedure to minimize the residual L phase saturation and the ultimate solvent retention inside the swept region. The average $x_{sl}^{edge}$ should be kept as high as possible throughout the whole process. The key point, however, is that to maintain a sufficiently high $x_{sl}^{edge}$ (requirement 1) requires sufficient amounts of solvent to be fed to the chamber which most likely will reduce the average chamber temperature. This is a counter-effect since it will limit the degree of displacement efficiency improvement and will result in a higher dynamic solvent retention inside the chamber due to impairment of requirement (2). This may be partially overcome by the coinjection procedure proposed by Keshavarz et al. (2014b). Their procedure was to start coinjection with high SSR, to achieve a sufficiently high $x_{sl}^{edge}$ as soon as possible. Then, SSR should be gradually decreased to avoid large quantities of solvent retained in situ. SSR reduction should be designed such that the average $x_{sl}^{edge}$ still stays in its desirable high range.

Pure steam injection is recommended for the final stage of the process to recover as much solvent retained in situ. SSR reduction should be designed such that the average $x_{sl}^{edge}$ is as high as possible when the solvent mole fraction in the injectant is increased to 0.16. This will result in a coinjection temperature of 203.7°C at an operating pressure of 2.000 kPa. Thus, the maximum temperature at the chamber edge will be 203.7°C which corresponds to a $x_{sl}^{edge,min}$ of 0.09 according to Figure 2.

Validation with Numerical Simulations

In this section, simple numerical simulations are performed using CMG’s thermal simulator STARS (CMG, 2013) to validate the model described in previous sections. A 2D reservoir model with a grid block size of 0.25 m, 500 m, and, 0.25 m in the x, y and, z directions, respectively, is considered. The STARS dynamic gridding option with an amalgamation block size of 4, 1 and 4 in the x, y and, z directions, respectively, and a 1°C tolerance condition on temperature is applied to improve the simulation run speed. Well spacing, horizontal well length, and reservoir thickness are 100 m, 500 m, and 20 m, respectively. The injector and producer are located at the left boundary of the reservoir at the depths of 14 m and 18 m, respectively. Thus, only one half of a symmetrical well pattern is simulated in this study. Homogeneous reservoir properties...
are given in Table 3. Identical relative permeability curves are used for SAGD and SA-SAGD simulations which are presented in Figure 7.

A single component bitumen with no initial gas to oil ratio is assumed in this study for simplicity. Properties of bitumen are similar to those presented in Tables 1 and 2. A bitumen viscosity-temperature relationship is given by Equation (12) (Mehrotra and Svrcek 1986):

\[ \ln \mu = \exp(A + B T) \]

(12)

where \( \mu \) is viscosity in cp and \( T \) is temperature in K. Constants \( A \) and \( B \) are 22.8515 and 3.5784, respectively. Pressure dependency of the bitumen viscosity is neglected in this study. Phase equilibrium calculations are based on composition independent K-value tables. STARS' default K-value table is used for the water component. K-value tables generated by Equation (A5) (see Appendix 1) and the constants presented in Table 1 are used for hydrocarbon components. Well constraints are also listed in Table 3. Capillarity and possibilities of mutual solubility of water and hydrocarbons and asphaltene precipitation are also neglected.

Initially \( C_5 \) with a constant concentration of 4 mol% is coinjected with steam. Here, each single gridblock corresponds to a CV described earlier in this work. Figure 8a shows the histories of temperature and solvent concentration in the \( L \) and \( V \) phases in gridblock (100,52) after the arrival of the chamber edge in \( C_5 \)-steam coinjection. Gridblock (1,1) is defined at the left-top corner of the model. The corresponding temperature of the gridblock gradually increases which results in partial evaporation of solvent. Figure 8b presents that the residual \( L \) phase saturation and solvent contents of the \( L \) and \( V \) phases will reduce as the gridblock is located deeper inside the chamber.

Figure 9 shows the profiles of temperature and the residual \( L \) phase saturation inside the chamber along the 52th row of the simulation (i.e., at a depth of 13 m from the model top) at 27 months from the start of simulation. The chamber edge is located at 29.25 m from the left boundary of the model. The \( L \) phase saturation shows a minimum at a distance of 26.25 m from the left boundary. The reason for higher residual \( L \) phase saturation in regions closer to the well pair is a lower historic peak solvent concentration in those regions; i.e., requirement 1 for displacement efficiency improvement has not been fully satisfied. The reason for a higher \( L \) phase saturation in regions closer to the chamber boundary is a lower temperature; i.e., requirement 2 for displacement efficiency improvement has not been fully satisfied. The \( L \) phase saturation in the regions closer to the chamber edge will further reduce as a result of a temperature increase upon further propagation of the chamber.

Table 4 summarizes the results obtained from numerical simulation and the results estimated by the mathematical model through Equations (9) and (10) for \( C_5 \)-steam coinjection with a constant SSR of 4 mol% at an operating pressure of 2,000 kPa. The last column of Table 4 shows the relative error in the estimations of model with respect to numerical simulation. The required input data for the mathematical model are presented in Table 5. Values of parameters in this table are similar to those used in or obtained from the numerical simulation. Estimations of the model are in reasonable agreement with the numerical simulation. Thus, the model has been capable of capturing the key mechanisms of displacement efficiency improvement.

Figure 10 compares the profiles of the residual \( L \) phase saturation, solvent mole fraction in the \( L \) and \( V \) phases and the temperature after 3 years and 9 months of simulation between two cases: one with a constant \( C_3 \) concentration of 4 mol% in the injectant and the other with a constant \( C_3 \) concentration of 16 mol% in the injectant. The red color in the profiles of the residual \( L \) phase saturation represents regions with an improved displacement efficiency beyond that of SAGD. Using a higher SSR expedites solvent accumulation at the chamber edge. This results in the local displacement efficiency improvement to be observed in regions closer to the well pair and the average \( L \) phase saturation inside the chamber to be lower.

Note that displacement efficiency has not been improved beyond that of SAGD, in regions closer to the side boundary of the reservoir, when a SSR of 16 mol% is used. The reason is that significant accumulation of solvent inside the chamber in these regions has prevented the temperature from rising up sufficiently even after this region is swept by the coinjection chamber (the counter-effect problem disused in an earlier section of this paper). The residual \( L \) phase consists of almost 100% solvent in this region.

Figure 11 shows the same profiles for another case in which the coinjection strategy recommended by Keshavarz et al. (2014b) has been followed. SSR of 16 mol% is used for one year after the pre-heating period. Then it follows a decreasing trend during the next four months and pure steam is injected afterwards. Using this coinjection strategy has kept the average \( s_{\text{edge}} \) in its high range during most of the chamber propagation period and has increased the average chamber temperature during the final period of the project compared to the cases with constant SSR. This, in turn, has improved the displacement efficiency beyond that of SAGD and partial recovery of the trapped solvent, even in regions closer to the side boundary of the reservoir model (Compare with Figure 10; \( S_L \) is approximately zero in these regions).

Table 6 compares the volume of displaced bitumen from within the coinjection chamber as well as the mole numbers of the retained solvent inside the chamber between the three simulation cases studied in this section. Using a varying SSR has considerably reduced the solvent retention in both the \( L \) and \( V \) phases inside the coinjection chamber.

Conclusions

This paper presented a mathematical procedure to model the displacement efficiency improvement during the SA-SAGD
process with a single component solvent for a dead-bitumen reservoir. The model is based on the interaction of solvent accumulation, temperature variation and phase equilibrium during co-injection. The key conclusions are as follows:

1. Unlike the current convention in the literature, i.e., modifying the end point saturations in the relative permeability curves, it was demonstrated that the experimentally observed displacement efficiency improvement during SA-SAGD can be explained and mathematically modeled by interaction of solvent distribution, temperature variation and phase behavior.

2. The two main mechanisms that contribute to the potential displacement efficiency improvement during SA-SAGD are: 1) sufficient solvent accumulation in the vicinity of the chamber interface and 2) phase transition as a result of temperature rise during further propagation of the chamber. Under the assumptions of this work, the first mechanism contributes to the ultimate bitumen recovery factor while the second mechanism contributes to solvent recovery. The absence or inefficiency of either of these two mechanisms impairs the displacement efficiency improvement.

3. Since the temperature and solvent concentration at the chamber edge are interdependent variables, the calculations are presented over the entire mixing line of bitumen and solvent. For a fixed solvent concentration at the chamber edge, the residual L phase saturation as well as the amount of solvent retention in both the L and V phases will reduce as the temperature increases; i.e., the accumulated solvent will gradually leave a specific CV of the reservoir medium towards the colder regions, as it is engulfed by the chamber.

4. Using a higher SSR expedites solvent accumulation near the chamber interface and improves the ultimate recovery factor of bitumen. However, continuous coinjection of a high concentration of solvent is likely to result in a lower chamber average temperature and a higher solvent retention in both the L and V phases, which may make the process uneconomical.

5. Estimations from the mathematical model were in reasonable agreement with results from numerical simulations. The improved knowledge obtained from the model can be utilized to design an optimum coinjection strategy in terms of displacement efficiency improvement as described by Keshavarz et al. (2014b). Such optimum design should allow for sufficiently high solvent accumulation at the chamber edge during chamber propagation as well as a sufficiently high chamber average temperature, particularly during the final stage of the process.

Acknowledgments
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Nomenclature
a,b,c: K-value correlation constants
C5: Normal pentane
Cij: Volumetric concentration of component i in phase j
Ki: K value of component i as defined by Equation A5
Kij: K value as defined by Equation A2
L: Oleic phase
Nij: Mole numbers of component i in phase j per pore volume of CV
Nc: mole numbers of the retained solvent within the coinjection chamber
P: Pressure
Pc: Critical pressure
P \text{\textit{ref}}: Reference condition pressure
P_{\text{\textit{sat}}}^i: Vapor pressure component i
Q.: Volume of bitumen displaced from within the chamber
R: Universal gas constant
S: Saturation
Slr: Residual L phase saturation
Slrg: Residual L phase saturation in the gas liquid system
Swi: Irreducible water saturation
T: Temperature
T_{\text{\textit{sat}}}^i: Saturation temperature of component i
Tc: Critical temperature
T_{\text{\textit{edge}}}: Chamber edge temperature
T_{\text{\textit{max}}}: Maximum chamber temperature
T_{\text{\textit{ref}}}: Reference condition temperature
T_{\text{\textit{avg}}}: Average chamber temperature
V: Gaseous phase
Vch: Chamber volume
$W$: aqueous phase

$x_{ij}$: Mole fraction of component $i$ in phase $j$

$x_{ij}^\text{edge}$: Mole fraction of component $i$ in phase $j$ at the chamber edge

$x_{\text{sl} \text{min}}$: Minimum mole fraction of solvent in the $L$ phase at the chamber edge

$z_i$: Overall composition of component $i$

$z$: Compressibility factor

$\alpha$: Compressibility

$\alpha_1$: First thermal expansion coefficients

$\alpha_2$: Second thermal expansion coefficients

$\omega$: Acentric factor

$\beta$: Phase mole fraction

$\phi$: Porosity

$\rho$: Molar density

$\rho_0$: Reference condition molar density in $L$ phase

**Subscripts and superscripts**

avg: Average

$i$: Component index

$j$: Phase index

$N_p$: Phase index for the reference phase

$o$: Bitumen component

$s$: Solvent component

$w$: Water component

**Abbreviations**

CV: Control volume

EOS: Equation of state

GCOS: Great Canadian oil sands

MW: Molecular weight

PR: Peng Robinson

RR: Rachford-Rice

SAGD: Steam-assisted gravity drainage

SA-SAGD: Solvent Aided-SAGD

SI: International system of units

SSR: Steam-Solvent coinjection ratio

**References**


TABLE 1. COMPONENTS USED IN PHASE EQUILIBRIUM CALCULATIONS

<table>
<thead>
<tr>
<th>Component</th>
<th>MW</th>
<th>(T_c, , ^\circ C)</th>
<th>(P_c, , \text{kPa})</th>
<th>(\omega)</th>
<th>(a, , \text{kPa})</th>
<th>(b, , ^\circ C)</th>
<th>(c, , ^\circ C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Water</td>
<td>18.01</td>
<td>374.15</td>
<td>22088.850</td>
<td>0.344</td>
<td>1.1860×10^7</td>
<td>-3816.44</td>
<td>-227.02</td>
</tr>
<tr>
<td>C_5</td>
<td>72.2</td>
<td>196.45</td>
<td>3374.120</td>
<td>0.251</td>
<td>1.0029×10^6</td>
<td>-2477.07</td>
<td>-233.21</td>
</tr>
<tr>
<td>Oil</td>
<td>594.6</td>
<td>817.75</td>
<td>785.980</td>
<td>1.361</td>
<td>where (P_0^{\text{vap}}) is calculated using PR EOS</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

TABLE 2. OIL AND SOLVENT DENSITY CORRELATION PARAMETERS USED IN PHASE SATURATION CALCULATIONS

<table>
<thead>
<tr>
<th>Component</th>
<th>(\rho_0, , \text{kgmol/m}^3)</th>
<th>(\alpha_c, , 1/\text{kPa})</th>
<th>(\alpha_s, , 1/\text{°C})</th>
<th>(\alpha_2, , 1/\text{°C}^2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C_5</td>
<td>8.736</td>
<td>1.69×10^-6</td>
<td>1.045×10^{-3}</td>
<td>2.82×10^{-6}</td>
</tr>
<tr>
<td>Oil</td>
<td>1.806</td>
<td>3.24×10^{-7}</td>
<td>2.044×10^{-4}</td>
<td>6.31×10^{-7}</td>
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TABLE 3. INPUT DATA FOR NUMERICAL SIMULATIONS

<table>
<thead>
<tr>
<th>Properties</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>33%</td>
</tr>
<tr>
<td>Horizontal permeability</td>
<td>4,000 md</td>
</tr>
<tr>
<td>Vertical permeability</td>
<td>3,000 md</td>
</tr>
<tr>
<td>Initial reservoir pressure at depth of 500 m</td>
<td>1,500 kPa</td>
</tr>
<tr>
<td>Initial reservoir temperature</td>
<td>13°C</td>
</tr>
<tr>
<td>Initial oil saturation</td>
<td>0.75</td>
</tr>
<tr>
<td>Initial water saturation</td>
<td>0.25</td>
</tr>
<tr>
<td>Three-phase relative permeability model (CMG, 2013)</td>
<td>Stone’s model II</td>
</tr>
<tr>
<td>Formation compressibility</td>
<td>1.8E-5 1/kPa</td>
</tr>
<tr>
<td>Rock heat capacity (Butler, 1997)</td>
<td>2,600 kJ/m³ °C</td>
</tr>
<tr>
<td>Rock thermal conductivity (Butler, 1997)</td>
<td>660 kJ/m day °C</td>
</tr>
<tr>
<td>Over/underburden heat capacity (Butler, 1997)</td>
<td>2,600 kJ/m³ °C</td>
</tr>
<tr>
<td>Over/underburden thermal conductivity (Butler, 1997)</td>
<td>660 kJ/m day °C</td>
</tr>
<tr>
<td>Bitumen thermal conductivity (Butler, 1997)</td>
<td>11.5 kJ/m day °C</td>
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<tr>
<td>Gas thermal conductivity (Yazdani et al., 2011)</td>
<td>2.89 kJ/m day °C</td>
</tr>
<tr>
<td>Water thermal conductivity</td>
<td>50.1 kJ/m day °C</td>
</tr>
<tr>
<td>Injector bottom-hole pressure (maximum)</td>
<td>2,000 kPa</td>
</tr>
<tr>
<td>Producer bottom-hole pressure (minimum)</td>
<td>1,500 kPa</td>
</tr>
<tr>
<td>Producer steam flow rate (maximum)</td>
<td>1 m³</td>
</tr>
<tr>
<td>Producer surface liquid rate (maximum)</td>
<td>2,000 m³/day</td>
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<tr>
<td>Steam quality</td>
<td>0.9</td>
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TABLE 4. COMPARISON OF RESULTS OF THE MODEL AND NUMERICAL SIMULATION

<table>
<thead>
<tr>
<th></th>
<th>Simulation</th>
<th>Model</th>
<th>Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Displaced bitumen (m$^3$)</td>
<td>86,836.90</td>
<td>86,925.77</td>
<td>0.1</td>
</tr>
<tr>
<td>Solvent retained in the L phase (mole)</td>
<td>5,620.77</td>
<td>5,385.12</td>
<td>-4.2</td>
</tr>
<tr>
<td>Solvent retained in the V phase (mole)</td>
<td>15,982.22</td>
<td>17110.17</td>
<td>7.0</td>
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TABLE 5. INPUT DATA FOR THE MATHEMATICAL MODEL

<table>
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<tr>
<th>Properties</th>
<th>Values</th>
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</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>33%</td>
</tr>
<tr>
<td>Chamber volume (m$^3$)</td>
<td>385,781.3</td>
</tr>
<tr>
<td>Average $x_{sL}^{edge}$ during chamber propagation</td>
<td>0.80</td>
</tr>
<tr>
<td>SSR (mol%)</td>
<td>4.0</td>
</tr>
<tr>
<td>Operating pressure (kPa)</td>
<td>2,000</td>
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TABLE 6. COMPARISON OF RESULTS OF THE THREE NUMERICAL SIMULATION CASES

<table>
<thead>
<tr>
<th></th>
<th>Constant SSR (4 mol%)</th>
<th>Constant SSR (16 mol%)</th>
<th>Varying SSR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chamber Volume (m$^3$)</td>
<td>385,781.3</td>
<td>385,968.8</td>
<td>385,250</td>
</tr>
<tr>
<td>Displaced bitumen (m$^3$)</td>
<td>86,836.9</td>
<td>90,768.75</td>
<td>89,156.33</td>
</tr>
<tr>
<td>Solvent retained in the L phase (mol)</td>
<td>5,620.77</td>
<td>21,543.78</td>
<td>1,557.084</td>
</tr>
<tr>
<td>Solvent retained in the V phase (mol)</td>
<td>15,982.22</td>
<td>25,396.79</td>
<td>5,372.149</td>
</tr>
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</table>
Figure 1. Tie triangle for ternary mixtures of water, solvent, and oil at a given pressure and temperature. Overall composition A is on the W-L edge of the tie triangle and represents a condition at the chamber edge. Overall composition B is in the three-phase region and represents a condition inside the coinjection chamber (Keshavarz et al. 2014c).

Figure 2. Solvent concentration in the equilibrium L and V phases within and at the boundary of the coinjection chamber. Operating pressure is 2,000 kPa. Solvent is C₅ and the reservoir oil is a gas-free Athabasca bitumen. Properties of components are listed in Table 1.
Figure 3. Variation of the residual oil saturation over the $x_{SL}^{edge}$-$T$ plane at 2,000 kPa. The reservoir oil is a gas-free Athabasca bitumen and the coinjected solvent is C$_5$. The $x_{SL}^{edge}$-axis shows the possible solvent concentrations in the L phase upon the arrival of the chamber edge to the CV. The $T$-axis represents the temperature after the chamber engulfs the CV. Since $T_{edge}$ and $x_{SL}^{edge}$ are interdependent, the temperature interval spans along the $x_{SL}^{edge}$ axis.
Figure 5. Average values of residual oil saturation and solvent retention in the $L$ and $V$ phases (per pore volume of CV) inside the coinjection chamber. Values are plotted along the solvent-bitumen mixing line at the chamber edge. The reservoir oil is a gas-free Athabasca bitumen and the coinjected solvent is $C_5$. For a fixed $x_{SL}^{edge}$, solvent retention in both $L$ and $V$ phases will decrease as the temperature of CV increases.
Figure 6. Average values of residual oil saturation and solvent retention in the \( L \) and \( V \) phases (per pore volume of CV) inside the coinjection chamber. Values are plotted along the solvent-bitumen mixing line at the chamber edge. The reservoir oil is a gas-free Athabasca bitumen and the coinjected solvent is \( C_5 \) with a molar concentration of 16\% in the injectant, at an operating pressure of 2,000 kPa. The average values are evaluated at the temperature estimated by Equation 8. The maximum temperature at the edge will be 203.7\( ^\circ \text{C} \), which corresponds to a \( x_{sl}^{edge} \) of 0.09.
Figure 7. Relative permeability curves used in the simulation cases; (a) the water-oil system and (b) the liquid-gas system.
Figure 8. Histories of (a) temperature and solvent concentration in the $L$ and $V$ phases and, (b) $L$ phase saturation and solvent retention in $L$ and $V$ phases for gridblock (100,52) after the arrival of chamber interface. Solvent concentration, $L$ phase saturation and solvent retention in both $L$ and $V$ phases will gradually reduce as the temperature of the gridblock increases.
Figure 9. Profiles of temperature and $L$ phase saturation of the swept region in the 13th row of simulation at 27 months. Chamber edge is located at a distance of 29.25 m from the left boundary. Temperature continuously decreases along the distance from the left boundary. $L$ phase saturation shows a minimum at a distance of 26.25 m from the left boundary, where both requirements 1 and 2 contribute efficiently to improve the local displacement of the $L$ phase.
Figure 10. Profiles of (a) residual $L$ phase saturation; (b) solvent concentration in the $L$ phase; (c) solvent concentration in the $V$ phase; and, (d) temperature, after 3 years and 9 months of C$_5$-steam coinjection simulation. A constant SSR is used throughout the simulations. Profiles on the left represent SSR of 4 mol% and profiles on the right represent SSR of 16 mol%. Regions in red in Figure 10a represent improvement of displacement efficiency beyond that of SAGD. Using a higher SSR improves the displacement efficiency in near wellbore region; however, it results in lower temperature close to the side boundary of the reservoir model which impairs the potential displacement efficiency improvement in this region. The $L$ phase in this region is composed of almost 100% solvent.
Figure 11. Profiles of (a) residual L phase saturation; (b) solvent concentration in the L phase; (c) solvent concentration in the V phase; and, (d) temperature after 3 years and 9 months of C₃-steam coinjection simulation. A constant SSR of 16 mol% is used during the first year. Coinjection continues with a declining SSR in the next 4 months, followed by pure steam injection afterwards. Implementing this coinjection strategy increases the average chamber temperature during the final period of the project resulting in higher bitumen displacement and solvent recovery from within the chamber.
Appendix 1

Equations used for phase equilibrium calculations are presented in this appendix. Based on assumptions (1) to (4) for phase equilibrium calculations, for a prescribed pressure (P) and temperature (T), the equilibrium phases’ compositions can be found by solving the following system of equations:

\[
P_i^{\text{sat}} = x_{wv} P \\
x_{oL} P_i^{\text{sat}} = x_{ov} P \\
x_{sL} P_s^{\text{sat}} = x_{sv} P \\
x_{oL} + x_{sL} = 1.0 \\
x_{wv} + x_{ov} + x_{sv} = 1.0
\] .................................(A1)

where water, oil and solvent components are labeled with indices \( i = w, o \) and \( s \) and aqueous, oleic and gaseous phases are labeled with indices \( j = W, L \) and \( V \), respectively. \( x_{ij} \) is the mole fraction of component \( i \) in phase \( j \) and \( P_i^{\text{sat}} \) is the vapor pressure of component \( i \).

Components’ partitioning between phases is expressed by K-values:

\[
K_{ij} = \frac{x_{ij}}{x_{iN_p}}
\] .................................(A2)

where \( x_{iN_p} \) is the mole fraction of component \( i \) in a reference phase, \( N_p \). With K-values and the overall composition \( (z_i) \) specified, the Rachford-Rice (RR) equations can be solved to give equilibrium phases’ mole fractions \( (\beta_j) \):

\[
f_j(\beta) = \sum_{i=1}^{3} \frac{(1-K_{ij})x_i}{1-\sum_{j=1}^{3}(1-K_{ij})\beta_j} \] .................................(A3)

with a constraint: \( \sum_{j=1}^{3}\beta_j = 1.0 \). The equilibrium phase compositions would be immediately calculated from:

\[
x_{iN_p} = \frac{x_i}{\sum_{j=1}^{3}(1-K_{ij})\beta_j} \\
x_{ij} = K_{ij}x_{iN_p} \quad (j \neq N_p).
\] .................................(A4)

K-values are estimated using the following correlation:

\[
K_i(P, T) = \frac{P_i^{\text{sat}}}{P} = a \times \frac{b}{P} \times e^{\frac{c}{T}}
\] .................................(A5)

where constants \( a, b \) and \( c \) are taken from Reid et al. (1977) and listed in Table 1. Vapor pressure of bitumen is calculated by the Peng-Robinson (PR) equation of state (1976). Note that based on the chosen reference phase \( (N_p) \), appropriate transformation of variables may be required before K-values defined in Equation (A5) can be substituted in Equations (A3) and (A4). More accurate results can be obtained if an equation of state (such as the PR equation of state) is used to generate K-values and to perform phase equilibrium calculations.