Scientific Contributions Oil & Gas, Vol. 48. No. 1, April: 1 - 10

SCIENTIFIC CONTRIBUTIONS OIL AND GAS
Testing Center for Oil and Gas
LEMIGAS

Journal Homepage:http://www.journal.lemigas.esdm.go.id
ISSN: 2089-3361, e-ISSN: 2541-0520

Improving Hydrocarbon Residue Feed Definition Through Validated Simulation Models

Rinzan Akhirjulima, IGBN Makertihartha, Tri Partono Adhi and Anggit Raksajati

Department of Chemical Engineering, Institut Teknologi Bandung
Labtek X Building, Ganesha Street, Bandung, 40132, Indonesia

Corresponding author: tpadhi@itb.ac.id

Manuscript received: October 21th, 2024; Revised: November 28th, 2024
Approved: December 09th, 2024; Available online: April 01th, 2025.

ABSTRACT - The conventional development of deasphalting processes is significantly dependent on costly and time-consuming lab experiments. Therefore, this study aimed to introduce a more efficient method using simulation to tackle the challenges associated with deasphalting. The method was used to identify the composition of synthetic crude oil (SCO) feedstock, dividing into 4 key molecular groups, namely Saturates, Aromatics, Resins, and Asphaltenes (SARA). These groups were pseudo-components in the simulation, characterized by parameters such as boiling points and molecular weights. The simulated boiling points were compared with actual crude oil to ensure accuracy. The framework was applied to model hydrocarbon residue in Lube Oil production, testing adaptability across various feedstocks. The strategy to improve the simulation accuracy was adjusting molecular interactions for asphaltene separation and refining pseudo-components. The results showed a boiling point curve with an RMSD of 2.689, closely matching the actual residue curve. This method improved the precision of deasphalting while reducing dependence on resource-heavy lab work.

Keywords: deasphalting, SARA molecule, simulation-generated boiling points curve, molecular interaction.

How to cite this article:

Rinzan Akhirjulima, IGBN Makertihartha, Tri Partono Adhi and Anggit Raksajati, 2025, Improving Hydrocarbon Residue Feed Definition Through Validated Simulation Models, Scientific Contributions Oil and Gas, 48 (1) pp. 1-10. DOI.org/10.29017/scog.v48i1.1683.

INTRODUCTION

Solvent deasphalting is an extraction process based on precipitation, occurring from changes in composition. This method uses solvents such as n-alkanes to precipitate paraffins. Lube Base Oil (LBO) widely uses solvent deasphalting to produce paraffinic raffinate, known as Deasphalted Oil (DAO) (Sequiera 1994). It also refines residual oil, generating raffinate products for hydrocracking or catalytic cracking (Corscaden et al. 2013). Extracts can be further processed into bitumen, coke, syngas, and other fuels. Typical solvents for extracting synthetic crude oil (SCO) from rock bitumen include toluene, formic acid, and surfactants such as dodecyl

trimethyl ammonium bromide (DTAB) (Sismartono et al. 2023). Solvents such as n-alkanes are also used in the deasphalting process to upgrade heavy crude oil for separating metals including nickel and vanadium (Carillo & Corredor 2013).

Generally, solvent deasphalting process starts with purifying heavy oils and metal residues, such as vanadium, which are detrimental to hydrocracking or hydrotreating processes. (Wilson et al. 1936) developed the foundational phase equilibrium model for processing heavy oils using propane as a solvent in dewaxing, deasphalting, and other refining processes. This model shows the development of propane deasphalting unit processes within LBO production. Although propane is widely used for selectivity in deasphalting process, solvents such as iso-butane and n-butane are more suitable for high-viscosity hydrocarbon materials due to their higher critical temperature values (Speight 2011).

A key challenge in developing the solvent deasphalting process is optimizing the separation of asphaltenes in semi-solid heavy hydrocarbon feedstocks, which range from 10% to 35% (Widarsono et al. 2023). These asphaltenes have high boiling points and viscosities, creating tar-like hydrocarbons trapped in porous rocks.Hydrocarbons extracted from mineral rocks use an advanced closed-loop extraction technology developed by Utah Oil Sands. This technology has an exceptionally high solvent recovery rate of approximately 99.9%. The method significantly mitigates environmental risks by eliminating the generation of slurry tailing ponds, a common byproduct in conventional extraction methods (Usman et al. 2019).

The more advanced method for solvent deasphalting has been successfully applied in the separation and granulation of asphaltenes, a process termed Supercritical Fluid Selective for Asphaltene Extraction (SELEX-Asp), using supercritical pentane as the solvent medium (Shi et al. 2007).

Heavy hydrocarbon upgrading using solvents starts with laboratory experiments assessing the extraction process for a specific hydrocarbon feedstock (HF) due to variability in feedstock composition. Although simulation experiments exist, their application is limited to the feedstock used in models. Changes in feedstock composition can compromise the deasphalting extraction process. This shows the need for further laboratory testing, which incurs significant time, labor, and financial costs. The initial step in developing a deasphalting simulation model is defining the feedstock compositional distribution, which varies based on a raw material source. This is followed by accurate modeling of the molecular interactions that govern asphaltene separation and precipitation, typically guided by boiling point curve data. In a study by (De Las Heras 2022), the deasphalting process was modeled using SARA (Saturates, Aromatics, Resins, and Asphaltenes) content data derived from a crude oil sample. This SARA-based crude oil was classified as SCO due to the representation as a pseudo-component set, each divided into several molecular categories. The pseudo-components were characterized by their estimated boiling points, molecular weights, and structural attributes. A boiling point curve was generated using these data and process simulation software (Aspen Plus). This curve was validated against boiling point data obtained from actual crude oil samples, as shown in the accompanying figure.

SARA content and boiling point curve analysis of heavy hydrocarbons are essential for characterizing their properties. It is generally assessed through thin-layer chromatography while boiling point distribution is determined using the SIMDIS method (Lee et al. 2014).

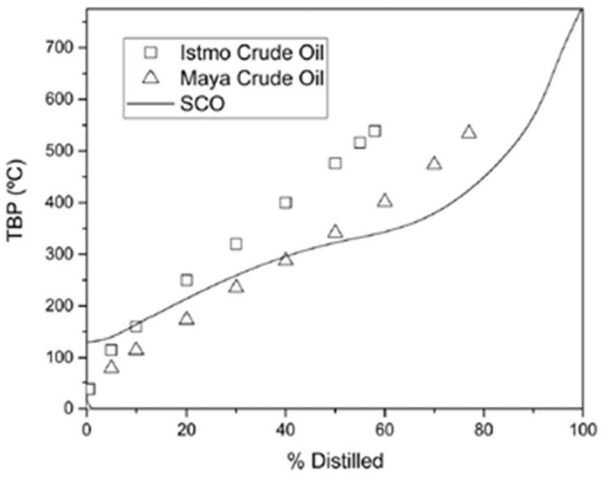

Figure 1
Boiling point curve comparison of SCO and actual crude oil

Modifications or adjustments were not made in developing the model to produce an SCO boiling point curve that closely replicated actual crude oil. Therefore, this study aimed to optimize the results generated by simulation software, refining the boiling point curve to more accurately show the properties of actual crude oil or short-chain residue oil.

Material

SCO composition was determined in the reference modeling process using SARA content data derived from crude oil samples, specifically Maya and Istmo Crude Oil (De Las Heras et al. 2022). The crude oil SARA composition, comprising 30% Saturates, 50% Aromatics, 5% Resins, and 15% Asphaltenes, was approximated into pseudo-components. These composition were further subdivided into 30 molecular entities, comprising 9 Saturates, 10 Aromatic, 5 Resin, and 6 Asphaltene molecules.

As shown in Figure 2, the SCO has a maximum boiling point of 756°C but the existing model formulation can only reach a temperature of 550.5°C. Therefore, compounds with boiling points ranging from 550.5°C to 756°C are treated as hypothetical within the simulation framework.

Table 1
Physical properties pseudo-component of SCO (De Las Heras et al. 2022)

Group Component	Molecules	Boiling Point (°C)	Molecular Weight (g/mol)
Saturate	1	133.5	114.2
	2	164.8	128.3
	3	167.8	140.0
	4	236.9	212.0
	5	277.6	252.0
	6	278.9	254.0
	7	321.8	282.6
	8	369.4	381.0
	9	404.9	422.8
Aromatic	1	138.2	106.2
	2	222.0	176.0
	3	234.8	174.3
	4	297.9	212.3
	5	308.4	256.4
	6	315.7	270.4
	7	319.0	240.4
	8	326.6	238.4
	9	347.2	298.0
	10	350.9	314.0
Resin	1	354.9	312.0
	2	407.6	400.6
	3	427.0	454.7
	4	447.0	490.0
	5	465.4	504.8
Asphaltene	1	502.8	588.9
	2	516.5	564.8
	3	521.3	638.9
	4	524.8	626.0
	5	527.6	607.0
	6	550.5	719.0

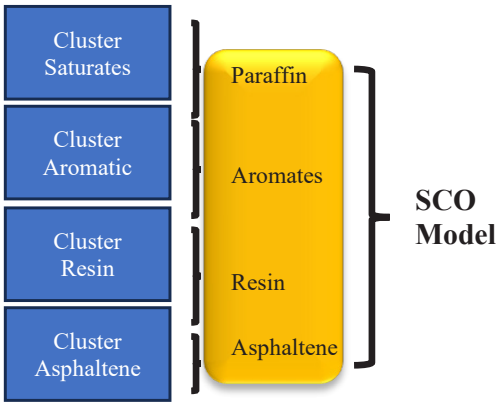

Figure 2
The diagram to identify the SCO composition in the form of pseudo-components

As shown in Figure 3, Process Flow Diagram (PFD) is used to determine the composition of SCO compounds accurately. This PFD facilitates the identification of compound composition by dividing each component (Normal Boiling Points at low temperatures), as well as the hypothetical components (Normal Boiling Points at high temperatures), into distinct flow streams, as shown in Tables 1 and 2. Subsequently, the flow of each component is calculated using the optimizer feature. This enables the precise determination of the SCO compound composition.

METHODOLOGY

The initial step in this study includes preparing pseudo-synthetic raw material feed components, using the SARA molecular group method presented in Table 1. The table provides molecular weight and boiling point data, while Table 2 shows the molecular structure information. These data are subsequently input into the Aspen HYSYS simulation software for component determination. The simulation methodology is systematically divided into 4 key components, namely the overall simulation process, the model validation method for

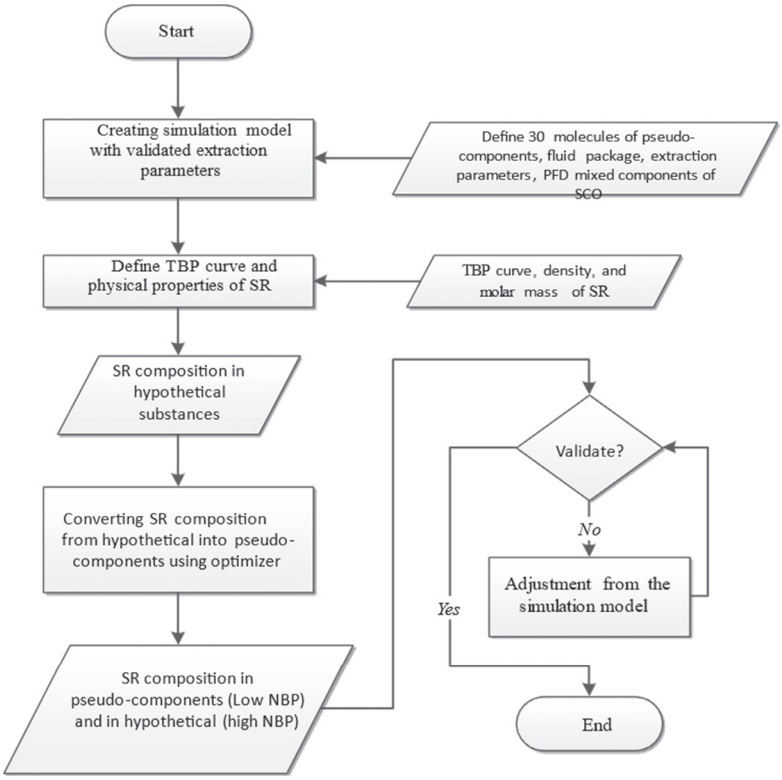

Figure 3
SCO characteristic validation method

identifying extraction parameters, the short residue (SR) characteristics validation, and the validation of the model against the actual system. A flow diagram representing the simulation methodology for SR characteristics validation is conducted using Aspen HYSYS, incorporating prior simulation models and SR characteristic data obtained from PT Pertamina. The flow diagram for the SR characteristic validation methodology is shown in Figure 4. SCO characteristics were validated using actual residual oil data samples within the Aspen HYSYS framework. The accompanying figure presents the flow diagram representing the validation method for the actual system.

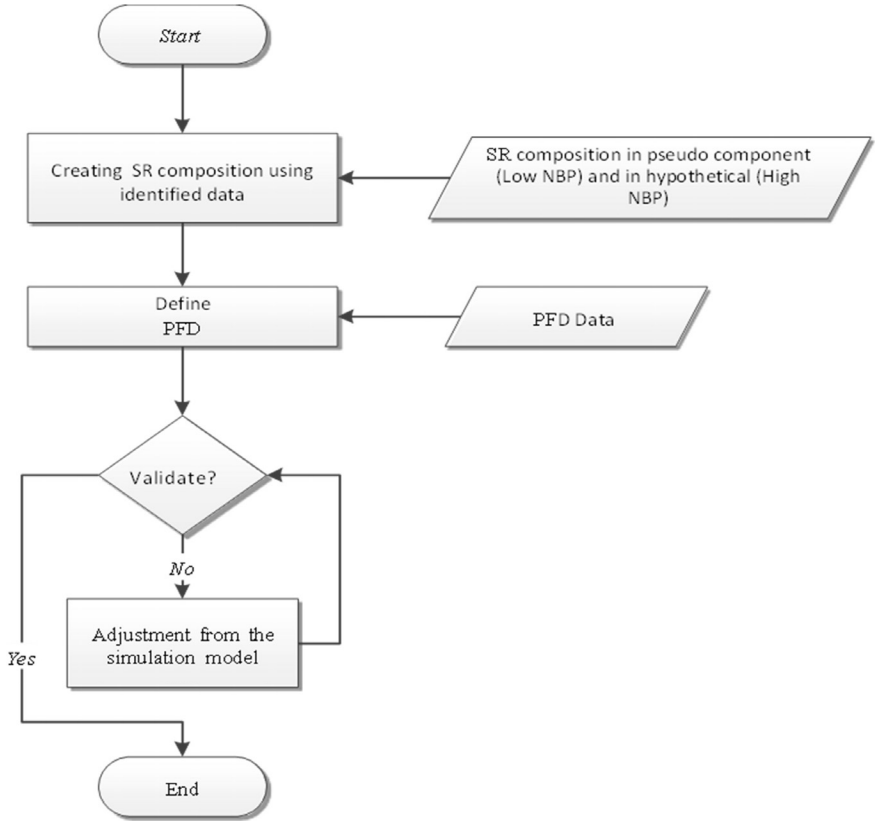

Figure 4
Actual system validation method

Table 2
Composition of SCO compounds after conversion in pseudo-component form

Component	Mole Fraction	Component	Mole Fraction	Component	Mole Fraction
Saturates-1	0.0662	Aromatics-4	0.0661	Asphaltenes-1	0.0328
Saturates-2	0.0125	Aromatics-5	0.0001	Asphaltenes-2	0.0035
Saturates-3	0.0128	Aromatics-6	0.0022	Asphaltenes-3	0.0017
Saturates-4	0/0000	Aromatics-7	0.0143	Asphaltenes-4	0.0016
Saturates-5	0.0562	Aromatics-8	0.0109	Asphaltenes-5	0.0074
Saturates-6	0.0388	Aromatics-9	0.0427	Asphaltenes-6	0.0173
Saturates-7	0.1083	Aromatics-10	0.0000	NBP 579	0.0153

Table 2 (continued)
Composition of SCO compounds after conversion in pseudo-component form

Component	Mole Fraction	Component	Mole Fraction	Component	Mole Fraction
Saturates-8	0.0522	Resins-1	0.0268	NBP 607	0.0126
Saturates-9	0.0000	Resins-2	0.0760	NBP 635	0.0111
Aromatics-1	0.0362	Resins-3	0.0162	NBP 673	0.0191
Aromatics-2	0.1362	Resins-4	0.0001	NBP 720	0.0201
Aromatics-3	0.0280	Resins-5	0.0402	NBP 769	0.0186

RESULT AND DISCUSSION

Table 2 shows the results of SCO compound composition, expressed as pseudo-components. This composition was subsequently revalidated against the True Boiling Point (TBP) curve, as shown in Figure 5. The TBP values are in line with the simulation results obtained from Aspen HYSYS and the SCO model proposed by (De Las Heras et al. 2022). Therefore, the developed model is considered suitable for the next stage, which includes validating SR characteristics. The process for validating SR characteristics differs from the model used in identifying extraction parameters, specifically through the application of PFD, as shown in Figure 4. The feedstock used is SR of the Arabian Light Crude (ALC) type, with specifications provided in Table 3. The target product, Deasphalted Oil (DAO), is asphalt with specifications presented in Tables 4 and 5. Table 4 shows the calculated composition of SR compounds as pseudo-components. A comparative analysis shows differences in the components attributed to the compositional variations between SCO and SR. The compositions detailed in Table 5 were further revalidated for conformity with the TBP curve of SR, as shown in Figure 6. The validated TBP curve strongly correlated with the Aspen HYSYS simulation results and the actual SR model. Therefore, the developed model provides a more accurate representation of the characteristics of an actual oil sample compared to previous simulation model methods. The enhanced model provides the best similarity result of TBP curve to the actual SR with a root mean square deviation (RMSD) of the mean boiling point curve of 2.689.

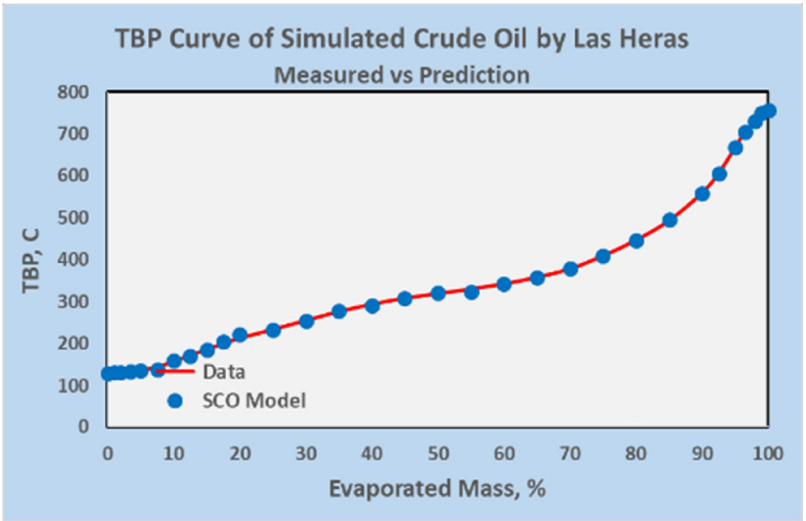

Figure 5
Comparison of TBP curves from simulation results with literature data

 | DOI.org/10.29017/scog.v48i1.1683

Table 3
Typical value of actual SR from lube base oil plant in Indonesia

Description	Value
Specific Gravity (@ 60/60oF)	1.0237
Viscosity @100ºF, CST	96296,1432
Viscosity @140ºF, CST	7581.3841
Viscosity @210ºF, CST	463.9728
UOP K Factor	11.4459
Refractive Index @20ºC	1.5775
Sulfur, %wt	4.1237
Wax, %wt	2.5031
Aniline Point, ºC	81.4880
Pour Point, ºC	36.2643
Flash Point (Measured Closed Cup), ºC	342.8921
Asphaltene, %wt	10.9923
Molecular Weight	742.9750
% Aromatic (ASTM D 3238)	42.9610
% Naphthenic (ASTM D 3238)	3.2059
% Paraffin (ASTM D 3238)	53.8331

Table 4
Typical value of boiling point distribution of actual SR measured by ASTM D 7169

Mass %	ºC	Mass %	ºC	Mass %	ºC	Mass %	ºC
IBP	455.4	26	544.4	52	593.0	78	650.2
1	469.2	27	546.2	53	594.8	79	652.8
2	480.2	28	548.2	54	596.8	80	655.4
3	486.8	29	550.0	55	598.8	81	658.0
4	492.0	30	552.0	56	600.8	82	660.8
5	496.2	31	553.8	57	602.8	83	663.6
6	499.8	32	555.8	58	604.8	84	666.4
7	503.0	33	557.6	59	607.0	85	669.4
8	506.0	34	559.4	60	609.0	86	672.4
9	508.8	35	561.2	61	611.2	87	675.4
10	511.4	36	563.0	62	613.4	88	678.6
11	514.0	37	564.8	63	615.6	89	681.8

Table 4 (contiued)
Typical value of boiling point distribution of actual SR measured by ASTM D 7169

Mass %	°C	Mass %	°C	Mass %	°C	Mass %	°C
12	516.4	38	568.4	64	617.6	90	685.2
13	518.6	39	570.0	65	619.8	91	688.6
14	520.8	40	570.2	66	622.0	92	692.0
15	523.0	41	572.0	67	624.2	93	695.2
16	525.2	42	574.0	68	626.4	94	698.4
17	527.2	43	575.8	69	628.6	95	701.6
18	529.2	44	577.8	70	631.0	96	704.8
19	531.0	45	579.6	71	633.2	97	708.2
20	533.0	46	581.6	72	635.6	98	711.6
21	535.0	47	583.6	73	638.0	99	715.6
22	536.8	48	585.4	74	640.4	FBP	717.6
23	538.8	49	587.2	75	642.8		
24	540.6	50	589.2	76	645.2		
25	542.6	51	591.0	77	647.6		

Table 5
Composition of SR substances after converted into pseudo-component.

Component	Mole Fraction	Component	Mole Fraction	Component	Mole Fraction
Resins-4	0.0001	NBP 494	0.0155	NBP 609	0.0450
Resins-5	0.0031	NBP 504	0.0215	NBP 619	0.0446
Asphaltenes-1	0.0276	NBP 511	0.0266	NBP 628	0.0423
Asphaltenes-2	0.0117	NBP 523	0.0309	NBP 638	0.0406
Asphaltenes-3	0.0000	NBP 532	0.0343	NBP 647	0.0386
Asphaltenes-4	0.0000	NBP 542	0.0351	NBP 657	0.0357
Asphaltenes-5	0.0292	NBP 551	0.0350	NBP 667	0.0333
Asphaltenes-6	0.0283	NBP 561	0.0534	NBP 676	0.0307
NBP 458	0.0022	NBP 571	0.0523	NBP 686	0.0285
NBP 465	0.0048	NBP 580	0.0500	NBP 696	0.0298
NBP 475	0.0061	NBP 590	0.0509	NBP 705	0.0284
NBP 485	0.0100	NBP 590	0.0485	NBP 714	0.0253

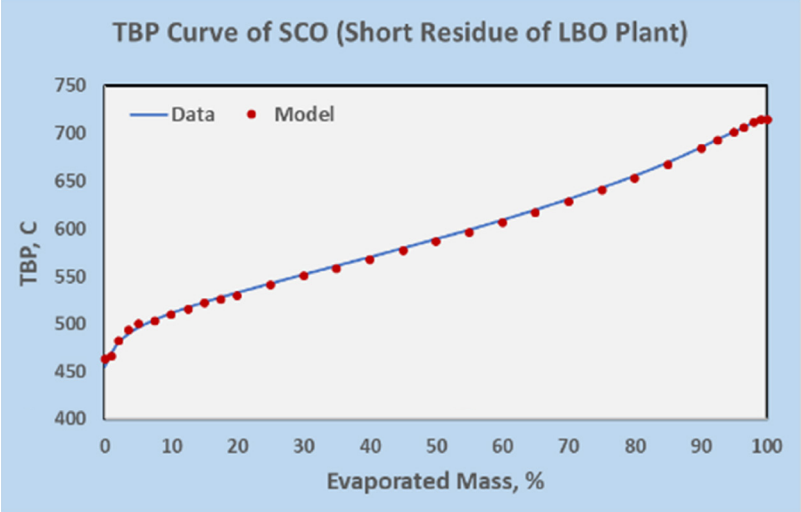

Figure 6
Comparison of TBP curves from simulation results with actual SR data

CONCLUSION

In conclusion, the simulation successfully produced a robust model for defining hydrocarbon residual oil materials. The results provided valuable information by comprehensively implementing the adopted methods. The SCO feed was defined using the model by (De Las Heras et al. 2022), which applied TBP curve data and bulk characteristics to derive the composition of hypothetical components. This was transformed into a pseudo-component framework of 30 compounds, comprising 9 Saturates, 10 Aromatics, 5 Resins, and 6 Asphaltenes.

The binary interaction properties of these pseudo-components were determined to simulate the extraction process accurately. Similarly, the SR feed obtained from lube oil plants was characterized using TBP curve data and bulk properties. This was converted into a pseudo-component framework based on the same methodology. The simulated TBP curve strongly correlated with the actual curve from laboratory tests by applying pseudo-component corrections and binary interaction adjustments. These results showed the effectiveness of the developed model in accurately characterizing hydrocarbon residual oils, offering a reliable tool for refining process simulations and optimizations.

ACKNOWLEDGMENT

PT Pertamina (Persero), Indonesia, funded this study through a postgraduate scholarship program and research and technology innovation funding.

GLOSSARY OF TERMS

Symbol	Definition	Unit
SCO	Synthetic Crude Oil	
SARA	Saturates, Aromatic, Resin Asphaltene	
LBO	Lube Base Oil	
DAO	Deasphalted Oil	
DTAB	Dodecyl Trimethyl Ammonium Bromide	
SELEX-Asp	Supercritical Fluid Selective for Asphaltene Extraction	
HF	Hydrocarbon	
SIMDIS	Feedstock	
Aspen Plus & Aspen HSYS	Simulated Distillation Simulation Software owned by Aspentech for Process simulation and optimization	
SR	Short Residue	
TBP	True Boiling Points	
ALC	Arabian Light Crude	
ASTM	American Society Testing Method	
RMSD	Root Mean Square Deviation	

REFERENCES

Sequeira, A., 1994, Lubricant Base Oil and Wax Processing. Marcel Dekker, New York.

Corscadden, T., Bruce, G., Diduch, G., Hocking, D. & Remesat, D., 2012, Enhanced methods for solvent deasphalting of hydrocarbons. World Intellectual Property Organization WO2013056361A1, filed August 3, 2012, and issued April 25.

Sismartono, D., Widarsono, B., Rahmadi, A., Usman, Akbar, W. A., Sunarjanto, D., Lubad, A. M., Herizal, Atmoko, A. D., Nurkamelia, Suhartono, R. & Kepies, S., 2023, Downstreaming Buton Asphalt Into Heavy Oil Production: A Techno-Economic Analysis Approach. Scientific Contributions Oil and Gas, Vol. 46, No. 3, pp. 1-19.

Carrillo, J.A. & Corredor, L.M., 2013, Upgrading of Heavy Crude Oils: Castilla. Fuel Processing Technology, 109, 1 May, 156–162.

Wilson, R.E., Keith, P.C. & Haylett, R.E., 1936, Liquid Propane: Use in Dewaxing, Deasphalting, and Refining Heavy Oils. Industrial & Engineering Chemistry, 28(9).

Speight, J.G., 2011, Chapter 7 - Deasphalting and Dewaxing Processes. In The Refinery of the Future (pp. 209–236). William Andrew Publishing, Boston.

Widarsono, B., Sunarjanto, D., Susantoro, T. M., Suliantara, Setiawan, H.L., Wahyudi, P., Sugihardjo, Romli, M. & Dwiyanarti, D., 2023, Integrated Approach to Investigate the Potential of Asphalt/Tar Sand on Buton Island, Indonesia. Scientific Contributions Oil and Gas, Vol. 46, No. 2, pp. 65-85.

Usman, Hazman, Pribadi, E., Lucia1, A. and Widarsono, B., 2019, Study of Regulation on Shallow Depth Oil Sands Business using Oil Mining Method. Lembaran Publikasi Minyak dan Gas Bumi, Vol. 53, No. 1, pp. 1-5.

Shi, Q., Zhao, S., Zhou, Y., Gao, J. & Xu, C., 2020, Development of Heavy Oil Upgrading Technologies in China. Reviews in Chemical Engineering, 36(1), January.

De Las Heras, I., Dufour, J. & Coto, B., 2022, Simulation of the Deasphalting Process of Crude Oils: Models Development and Extraction Conditions Analysis. Journal of Petroleum Science and Engineering, 208, 1 January.

Lee, J.M., Shin, S., Ahn, S., Chun, J.H., Lee, K.B., Mun, S., Jeon, S.G., Na, J.G. & Nho, N.S., 2014, Separation of Solvent and Deasphalted Oil for Solvent Deasphalting Process. Fuel Processing Technology, 119, 1 March, 204–210.