Q2 2025

ptq

REFINING
GAS PROCESSING
PETROCHEMICALS

CRUDE-TO-CHEMICALS

INCREASING WATER QUALITY

CORROSION INHIBITORS

ADVANCING CHEMICAL RECYCLING

Thermodynamic solution for evaluating crude compatibility

Case studies emphasise the power of advanced analytical tools such as predective modelling in crude compatibility assessment and blend management

Asok Tharanivasan and Michelle Wicmandy
KBC (A Yokogawa Company)

Global crude oil demand is projected to tip 103 million bpd in 2025, according to the International Energy Agency (IEA). As refiners aim to maximise output while keeping costs in check, many are turning to opportunity crudes from various geographical locations throughout the world. This shift presents the refining industry with challenges in optimising crude oil blends driven by the growing demand for diverse crude sources, stringent environmental regulations, and economic pressures. While opportunity crudes are economically attractive, they are unpredictable – you never know what you are going to get in terms of composition and properties.

One critical issue that refineries face when grappling with opportunity crudes is asphaltene stability. Specifically, this refers to how well the asphaltenes are dissolved in the crude oil at a given operating temperature and pressure in refinery processes. Asphaltenes, the heavy and complex molecules in crude oil, can precipitate to either remain suspended or settle, depending on the conditions. The presence of precipitated asphaltenes can alter the physical properties of the fluid stream, leading to fouling and equipment damage, which causes significant operational inefficiencies and increased maintenance and repair costs.[1]

Problem

Asphaltene precipitation, the precursor of asphaltene-related problems, is a thermodynamic phenomenon that depends on the fluid composition, temperature, and pressure. Additional factors such as the residence time, equipment configuration, chemical reactions, and high process temperatures can produce deposition in streamlines, pump plugging, and equipment fouling. Hence, asphaltene precipitation is the primary trigger for these issues.

Typically, refiners assess asphaltene precipitation in a particular crude oil using standardised titration tests. These tests determine the onset point, which represents the minimum amount of titrating solvent required to initiate asphaltene precipitation.

Usually, the onsets are reported in mL of solvent per g of oil. Alternatively, the onsets are also reported as P-Value (ASTM D7112[2], ASTM D8253[3]), P-Ratio (ASTM D7060[4]), and S-Value (ASTM D7157[5]). Wiehe[6] presents the measured onsets in terms of solubility blending number (SBN) and the insolubility number (IN).

The onset point indicates the severity of asphaltene precipitation; for instance, higher onset values indicate more stable crude oils. Crude oils containing precipitated asphaltenes are considered unstable, where the onset cannot be measured. Test conditions (pressure and temperature) and titrants, typically n-heptane and n-hexadecane, vary by procedure, with most tests conducted at ambient conditions. Notably, onset values do not correlate to bulk asphaltene content of the crude oil.

Blending crude oils from various sources is unavoidable during transportation, pre-refining, and refinery processing. Additionally, mixing processed fluid streams containing asphaltenes occurs during processing, and product streams are blended in certain scenarios during post-refining operations. In all these cases, the source oils are incompatible when blending compositionally different stable source oils that lead to asphaltene precipitation. Consequently, using the correct proportion of source oils is crucial to avoid any unstable blends while ensuring compatibility.

While onset tests assess blend compatibility, testing all possible blends is impractical and expensive. Simple averaging is unreliable, as asphaltene solubility depends on fluid composition. This underscores the need for a predictive tool to assess the compatibility of different source oils or streams. In today's fast-paced environment, seamless integration of such a predictive tool into a process simulator is vital for efficient planning and operations.

Solution

To address the crude oil compatibility challenges, a Multiflash Crude Compatibility Tool (MFCCT) was developed and incorporated into KBC's proprietary Petro-SIM process simulator. Adapted from KBC's proprietary Multiflash asphaltene model, the MFCCT predicts asphaltene precipitation onsets for blends, and it has been validated using data from several refineries. Its predictive capabilities eliminate the need for extensive measurements in identifying the extent of compatibility of source oils or streams. Since the tool is based on the thermodynamic model, compatibility assessments can be extended to changing operating conditions, providing a reliable and efficient solution for

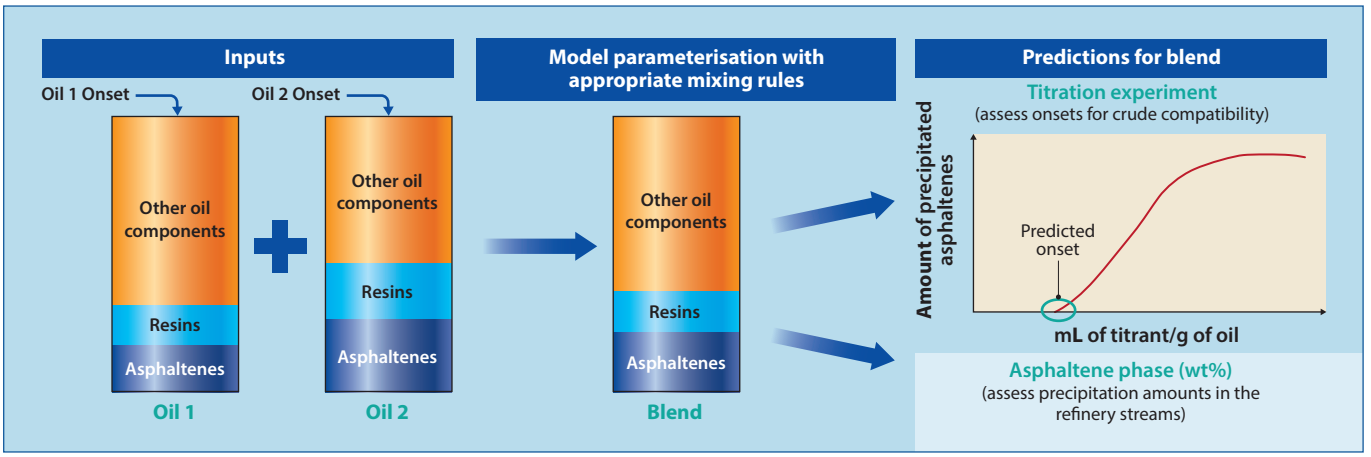

Figure 1 Flowchart of methodology to model asphaltene precipitation in oil blends

blending and process optimisation. This enables refiners to make informed decisions quickly and effectively.

Asphaltene model

At the core of the MFCCT is a robust thermodynamic framework that considers vapour, liquid, and asphaltene as equilibrium phases.[7] The model employs the cubic plus association equation of state (CPA-EOS) for phase equilibrium calculations. Asphaltene precipitation is modelled by considering two key mechanisms: asphaltene-asphaltene self-association and asphaltene-resin cross-association. At least one onset data is required to parameterise the model to account for the association behaviour of asphaltenes.

In terms of fluid characterisation, the refinery assay and the properties are represented as a defined number of pseudo-components, including the assignment of component properties for phase equilibrium calculations. The key steps involved in the characterisation are generating a boiling curve from the crude assay, translating the boiling curve into single carbon number (SCN) fractions, and lumping of SCN fractions into a specific number of pseudo-components using appropriate estimation methods and correlations. The inclusion of saturates, aromatics, resins, and asphaltenes (SARA) or paraffins, naphthenes, and aromatics (PNA) data will enhance the characterisation accuracy.

Note that this asphaltene phase behaviour model applies only to a single-source oil when calculating precipitation amounts upon dilution with a pure precipitating solvent (for example, n-heptane). When a source oil is blended with other source oils, the association behaviour and the solubility of asphaltenes are affected.

Adaptation of the model for oil blends

Figure 1 summarises the methodology used for phase behaviour modelling of oil blends. Fluid characterisation and parameterisation are first performed individually for each source oil. Each source oil requires a crude assay with asphaltene content and onset data. Simulated distillation data and bulk density are acceptable when full crude assay is absent.

Second, assays for the source oils are blended based on their proportions, followed by fluid characterisation. Third, model parameters for each source oil are blended using appropriate mixing rules to determine the blend's parameters. Finally, the phase equilibrium calculations use the characterised fluid and the blend parameters. The calculations simulate the titration experiment, thereby predicting the onset for the blend. If the blend is unstable, the precipitation amounts are calculated. Note that the Petro-SIM simulator automates these calculations once the source oil streams are defined.

MFCCT validation

Validation of the MFCCT was carried out using data from several refiners. A set of source oils was selected to measure their composition, properties, and onset data. These source oils were then blended in different proportions to create a select number of blends, for which the onsets were also measured.

All the source oil streams were set up and synthesised in the Petro-SIM software, including their onset data, to establish the parameters for each source oil. A product blend stream was then created using appropriate source oil proportions, together with normal refinery property blending rules and MFCCT mixing rules, to calculate its composition and properties, including the predicted onset if the blend was stable. If the blend was unstable, the amount of precipitation (asphaltene phase) was calculated. The predicted onset was validated by comparing it to the measured onsets.

Figure 2 compares predicted and measured onsets for blends of Oil 1 and Oil 2. Due to proprietary constraints, their composition and properties are not disclosed. Onsets for Oil 1 and Oil 2 were fitted, and blend onsets (Oil 1/Oil2 in wt%) at 75/25, 50/50, and 25/75 were predicted. The weight-averaged onsets for blends, based on source oil

Compatibility assessments based on the BCI

Range	Interpretation
BCI = 0.0	Incompatible source oil proportions
0.0 < BCI < 0.7	Potentially incompatible source oil proportions (prone to unstable stream with processing)
0.7 ≤ BCI < 1.0	Potentially compatible source oil proportions
BCI ≥ 1.0	Compatible source oil proportions

Table 1

onsets, were included for comparison. The non-linearity in the blend onsets was very well predicted by the model.

Such validation was conducted for more than 40 crude blends, including binary (two-source) and ternary (three-source) blends. The onset data for the source oils covered different titration solvents and temperatures ranging from 20°C to 150°C. Overall, MFCCT reported a high predictive accuracy with an average absolute deviation (AAD) of 0.17 mL/g. This result demonstrated its effectiveness in capturing the asphaltene phase behaviour of blends.

Compatibility assessment guidelines

Beyond onset predictions, a normalised measure called Blend Compatibility Index (BCI) has been developed to assess blend stability. This index provides a measure of non-linearity. Specifically, the index illustrates the blends' uniqueness when compared to the source oils in terms of asphaltene solubility. It is dimensionless and calculated at 60°F and 1 atm as the ratio of predicted onsets to the weight-averaged onset. A BCI value greater than zero indicates a stable blend, while a value of zero signals an unstable blend. **Table 1** provides an interpretation of BCI for blends.

By analysing crude blend stability using a structured compatibility index, the refineries can identify problematic combinations and optimise blending proportions. Further, BCI may offer insights into the preferred blending order of source crudes, though this aspect has not been assessed due to a lack of data.

Following are general compatibility assessment guidelines based on the tested datasets. These guidelines are subject to refinement as more data becomes available.

- **Low risk (onset ≥ 0.6; BCI > 0):** stable blend with compatible source oils.
- **High risk (0.2 < onset < 0.6; BCI > 0):** potentially stable blend and requires BCI analysis to identify problematic source oils
- **Not recommended (onset ≤ 0.2; BCI ≥ 0):** unstable blend and not advisable for processing.

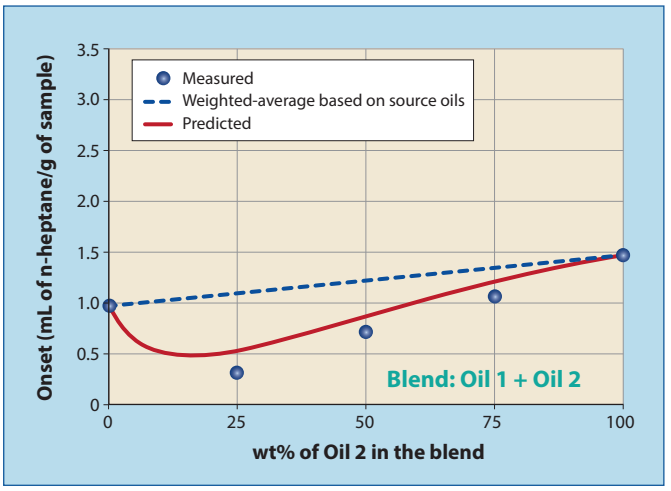

Figure 2 Predicted onsets compared against the measured onsets for Oil 1 and Oil 2 blends

Note that the onset values for the assessment are expressed in mL of n-heptane/g of sample. These guidelines are not established for other titrating solvents. However, BCI analysis can still be performed.

To illustrate the effectiveness of the MFCCT, the following case studies highlight different scenarios where crude compatibility assessments are evaluated by the refiners.

Case study 1

This case study involves data from a refiner who provided detailed source oil information, including the P-Value as the onset data. The dataset also included the proportions of six blends and their respective P-Values. The refiner's assessment classified these blends into three categories:

- Blend 1 was deemed acceptable for processing.
- Blends 2-5 were categorised as 'business-to-risk'.
- Blend 6 was determined unsuitable for processing.

MFCCT was used to independently evaluate these blends based on P-Value and the BCI. Note that P-Value = 1+onset in mL/g. As illustrated in **Table 2**, the tool's predictions aligned perfectly with the refinery's initial classification,

MFCCT predictions of P-Values alongside client data, demonstrating alignment between predicted and actual outcomes

Source crude	P-Value	Volume %					
		Blend 1	Blend 2	Blend 3	Blend 4	Blend 5	Blend 6
Crude 1	1.68	12.5	76	5	44	35	1
Crude 2	1.39	12.5	8	5	3	35	12
Crude 3	2.95	12.5	0	1.5	0	7	0.5
Crude 4	1.28	12.5	0	5	2	1.5	25
Crude 5	1.08	12.5	8	8	0	1.5	50
Crude 6	1.64	12.5	0	10	7	5	10
Crude 7	2.66	12.5	0	1.5	0	2	0.5
Crude 8	1.63	12.5	8	64	44	13	1
Refinery client	P-Value	1.64	1.58	1.40	1.46	1.40	1.18
	Assessment	Proceed	Business-to-risk				Not recommended
KBC (MFCCT)	P-Value	1.57	1.62	1.36	1.42	1.40	1.09
	BCI	0.69	1.03	0.60	0.66	0.59	0.35
	Assessment	Low risk		High risk			Not recommened
		Compatible		Potentially incompatible crude proportions			

Table 2

MFCCT predictions based on the SBN and IN data for source oils								
Source crude	SBN	IN	Volume %					
			Blend 7	Blend 8	Blend 9	Blend 10	Blend 11	Blend 12
Crude 9	63	31	53	52.9				
Crude 10	48	26	47	47		76		75
Crude 11	71	35					79	
Crude 12	73	32			17			18
Crude 13	50	35			83			
Crude 14	81	47		0.1		24	21	
Crude 15	30	0						7
Refinery client	SBN_{mix}		56	56	54	56	73	51
	IN_{max}		31	47	35	47	47	32
	Assessment		Compatible					
KBC (MFCCT)	Onset (mL/g)		1.01	1.01	0.62	0.74	1.02	1.00
	BCI		0.91	0.91	0.87	0.77	0.95	0.73
	Assessment		Low risk					
			Compatible crude proportions					

Table 3

reinforcing its reliability and accuracy to prepare the feed crude slate. This validation highlighted MFCCT's ability to replicate and enhance traditional blend evaluations.

Case study 2

The second case study is based on data from another refiner who provided full crude assays for seven source oils, including Wiehe's numbers (SBN and IN) as the onset data. Both SBN and IN are dimensionless values, and they are derived from Wiehe's proprietary titration methods conducted at 60°C. Specifically, SBN is determined from the heptane dilution test, whereas IN is obtained from the toluene equivalence test.

Table 3 presents the SBN and IN data, including the proportions of the six blends evaluated for the crude feed slate. The refiner's assessment on compatibility was based on SBN_{mix} and IN_{max}, depending on the volumetric proportions of source oils. As shown in Table 3, all six blends are considered stable, and the source oils are compatible per Wiehe's compatibility criterion ($SBN_{mix} > IN_{max}$).

MFCCT was independently applied to evaluate these six blends using the source oil data. For onset values, both SBN and IN were translated to a single onset in mL of n-heptane per g of sample for each source oil, enabling their use within the tool. This translation is performed automatically within the Petro-SIM simulator.

As shown in Table 3, MFCCT predicted that all blends were stable and compatible source oils, aligning with the refiner's or Wiehe's assessment. Additionally, MFCCT provided additional insights into blend stability. For instance, the predicted onsets for Blend 9 and Blend 10 were 0.62 and 0.74 mL/g, respectively. These are borderline values for classification as high risk, which was confirmed by the refiner based on their experience.

Key findings

Together, these case studies emphasise the power of advanced analytical tools in crude compatibility assessment and blend management. The case studies collectively highlight the value of advanced tools like MFCCT in assessing crude compatibility. Key findings include:

1. The tool's ability to predict blend onsets with high accuracy, preventing costly operational risks.
2. The development of the BCI, which quantifies non-linearity and provides actionable insights into crude compatibility.
3. The model accounted for the non-linearity of blend onsets, which traditional linear mixing rules often miscalculate, leading to operational risks.
4. More than 40 refinery blends were tested, validating the MFCCT tool's predictive capabilities.

Broader applications

MFCCT's predictive capabilities extend beyond compatibility analysis with applications across various refinery processes:

- **Planning and scheduling:** Supports crude selection and scheduling, enhancing flexibility for slate mixes and complementing linear programming models.
- **Crude storage and handling:** Assesses sludge build-up risks.
- **Processing:** Evaluates feeds for process units, such as desalters and preheat exchangers, and identifies fuel oil blend stability risks.

Conclusion

As the refining industry continues to navigate a rapidly evolving energy landscape, the MFCCT stands out as an essential solution for improving operational efficiency and reliability. By tackling the ongoing challenge of crude compatibility, MFCCT equips refiners with the insights they need to optimise operations, make informed decisions, and mitigate risks.

Opportunity crudes, though economically appealing, often bring unpredictable properties. This variability presents both challenges and opportunities. With its robust

thermodynamic model, MFCCT has consistently demonstrated reliable performance across diverse datasets, including crude oils and refinery streams. Its ability to accurately predict asphaltene precipitation allows refiners to identify stable blends, significantly cutting costs associated with trial-and-error testing. Furthermore, its integration with the Petro-SIM process simulator enhances planning and scheduling capabilities, providing refiners with a more comprehensive and efficient approach.

By combining predictive accuracy with seamless integration, MFCCT turns operational challenges into opportunities. It enables refiners to achieve immediate operational efficiencies while advancing long-term sustainability goals, aligning with the mission of Bringing Decarbonization to Life.

Acknowledgements

Mike Aylott, Merih Mustafa, Nuno Pedrosa, Xiaohong Zhang, and Richard Szczepanski, all from KBC (A Yokogawa Company), for the technical inputs and contributions in developing the tool. Extends the appreciation to all the refiners who supplied the datasets for validations and case studies.

References

1 Falkler, T., Sandu, C., Fine-tune processing heavy crudes in your facility, *Hydrocarbon Processing*, September 2010, pp67-73.
2 ASTM D7112, Standard test method for determining stability and compatibility of heavy fuel oils and crude oils by heavy fuel oil stability analyzer (optical detection), ASTM International, 2020.
3 ASTM D8253, Standard test method for determination of the asphaltene solvency properties of bitumen, crude oil, condensate and/or related products for the purpose of calculating stability, compatibility for blending, fouling, and processibility (Manual microscopy method), ASTM International, 2021.
4 ASTM D7060, Determination of the maximum flocculation ratio and peptizing power in residual and heavy fuel oils (Optical Detection Method), ASTM International, 2020.
5 ASTM D7157, Standard test method for determination of intrinsic stability of asphaltene-containing residues, heavy fuel oils, and crude oil (n-heptane phase separation; optical detection), ASTM International, 2020.
6 Wiehe, I. A., Asphaltene solubility and fluid compatibility, *Energy & Fuels* 26 (7), 2012, pp4004-4016.
7 Zhang, X., Pedrosa, N., Moorwood, T., Modeling asphaltene phase behavior: comparison of methods for flow assurance studies, *Energy Fuels*, 26 (5), 2012, pp2611-2620.

Asok Tharanivasan is an R&D Senior Consultant at KBC (A Yokogawa Company), specialising in asphaltene phase behaviour modelling and developing fluid property engines for process simulation tools. With 15 years in the oil industry, his expertise includes petroleum thermodynamics, hydrocarbon PVT phase behaviour, fluid characterisation, and flow assurance. Tharanivasan holds a PhD in chemical engineering and is a registered Professional Engineer in Alberta, Canada.

Michelle Wicmandy is Marketing Campaigns Manager at KBC (A Yokogawa Company) in Houston, Texas, with more than 20 years of experience in marketing and communications. She serves on the Forbes Communication Council and has contributed to both academic and trade publications. Wicmandy holds a DBA in business administration. *Email: michelle.wicmandy@kbc.global*