PLATFORM - A Journal of Science & Technology

Industrial Articles Presented in International Conference on Process Engineering and Advanced Materials (ICPEAM2020), 13-15 July 2021

APPLICATION OF PIONA CHARACTERISATION IN REFINERY PROCESS MODELING

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ABSTRACT

Refinery feed and product streams consist of a complex mixture of hydrocarbons ranging from C1 molecules to C200 and higher molecules depending on the fluid type (e.g., crude feed, kerosene products, Residue, etc.). The traditional approach to characterise the refinery fluid is by generating Pseudo-components based on the fluid laboratory analysis, mainly the boiling point range and the fluid bulk properties analysis. Although this approach to define the refinery process feeds and products can capture the required mass and energy balance to a certain extent, a much detailed analysis of the refinery fluid cannot be performed with a high degree of accuracy due to the inherent limitation in the traditional Pseudo-component definition approach. A case study on the new simulation approach was performed by defining the refinery fluid characterisation using the PIONA distribution methodology using a commercial process simulator. A comparison was made between traditional Pseudo-component characterisation vs. PIONA characterisation on the simulation results and calculated parameters. A significant improvement in simulated parameters was observed, contributing to higher accuracy in refinery process modelling. In addition, this new PIONA characterisation approach will support rigorous modelling of various refinery reactors for better reactor performance prediction.

Keywords: *Refinery Process Simulation, Refinery Fluid Characterisation, PIONA, Pseudo-component, Refinery Product Properties*

INTRODUCTION

Modelling Refinery Processes using a commercial process simulator poses significant challenges as the refinery feeds and product composition are highly complex. Refinery feed and product streams consist of a complex mixture of hydrocarbons ranging from C1 molecules to C200 and higher molecules depending on the fluid type (e.g., crude feed, kerosene products, Residue, etc.). The traditional approach to characterise the refinery fluid is by generating Pseudo-components based on the fluid laboratory analysis, mainly the boiling point range (TBP, D86, etc.) and the fluid bulk properties analysis. The basic idea represents the whole spectrum of the hydrocarbon mixture in the fluid with several hypothetical components defined by boiling points and densities based on the boiling point range. Although this approach to define the refinery process feeds and products can capture the required mass and energy balance to a certain extent, a much detailed analysis of the refinery fluid cannot be performed with a high degree of accuracy due to the inherent limitation in the traditional Pseudo-component definition approach. For example, the traditional Pseudo-components approach does not capture the various hydrocarbon molecules' structure (e.g., isomers, cyclic, aromatics, etc.) the various structure in a particular fluid is also not defined. This will lead to inaccuracies in calculating certain refinery fluid specifications (e.g. RON, Cetane Index, etc.) as the specification properties highly depend on the hydrocarbon molecules structure distribution.

MATERIALS AND METHODS

A case study on the new simulation approach was performed by defining the refinery fluid characterisation using the standard refinery fluid boiling point approach (Table 1) and PIONA distribution characterisation (Table 2) approach using the iCON Symmetry [1] process simulator.

Both fluid characterisations are configured in the simulator as shown in Figure 1, and the same set of operating conditions is used to flash the fluid to determine the properties and molecule distribution.

RESULTS AND DISCUSSION

A significant variation in simulated parameters was observed when the results of the stream flashing were compared. Physical properties, namely Molecular Weight, Enthalpy, Heat Capacity, and Viscosity, varied from 6% for Heat Capacity to 50% for Viscosity, as depicted in Figure 2. This can cause problems to equipment design, such as heat exchanger sizing.

Molecule distribution is also significantly varied. The estimated PIONA distribution from normal boiling point characterisation has more Naphthene and Aromatics

Table 1 Fluid boiling point analysis

PROPERTIES	UNITS	Heavy Design Case		Light Design Case	
TBP Cut Point	°C	C5 - 170		C5 - 170	
Flowrate	t/h	354.3		374.3	
specific gravity (60°F/60°F)	-	0.719		0.724	
Density	°API	65.4		64.0	
Distillation curve		TBP	ASTM D86	TBP	ASTM D86
IBP	°C	8	45	8	45
5 vol%	°C	32	61	32	61
10 vol%	°C	42	67	42	68
30 vol%	°C	83	92	83	92
50 vol%	°C	108	108	110	110
70 vol%	°C	134	127	133	126
90 vol%	°C	162	150	161	149
95 vol%	°C	171	157	170	156
FBP	°C	178	163	178	162

Table 2 Fluid PIONA analysis

Sulphur content	wt%	0.032	0.051
RVP	bar abs	0.30	0.30
Benzene	vol%	0.47	0.81
Pariffins	vol%	72.2	68.0
Olefins	vol%	0.0	0.0
Naphthenes	vol%	19.8	23.9
Aromatics	vol%	8,0	8.1
Metal (Fe+Va+Ni)	wt ppm	< 1	< 1
Nitrogen	wt ppm	< 1	< 1

Table 6.6.3: Stabilized Naphtha Properties

CCN	90% vol	°C	172	175	
	95% vol	°C	188	190	
	FBP	°C	206	206	
	C4	wt-%	0.50	0.49	
	Sulphur	wt-ppm	160	180	
	Paraffins	vol-%	29.2	19.8	
	Olefins	vol-%	37.5	41.2	
	Naphtenes	vol-%	6.6	5.6	
	Aromatics	vol-%	26.8	33.4	
	MAV		8	12	

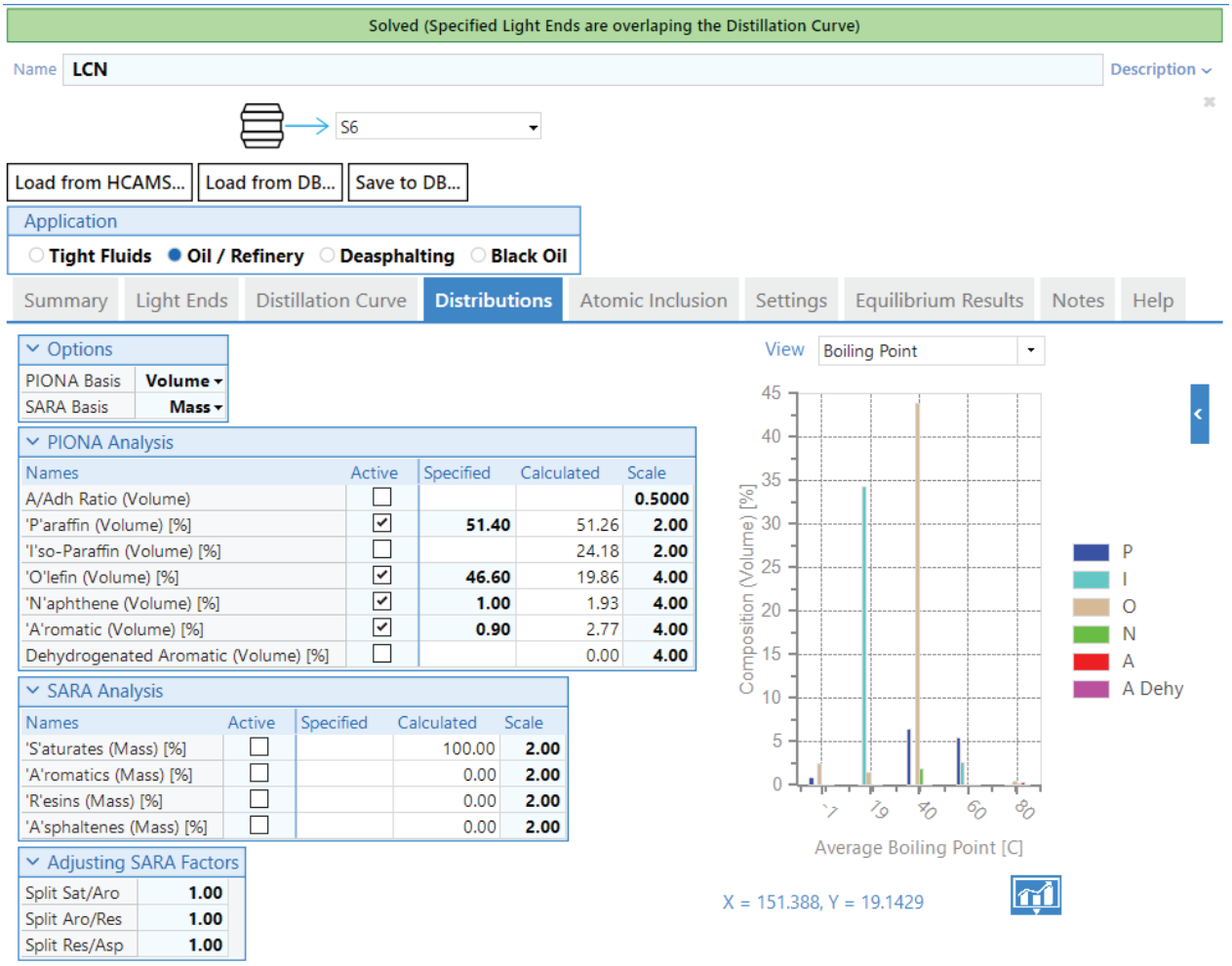

Figure 1 Fluid characterisation in simulator

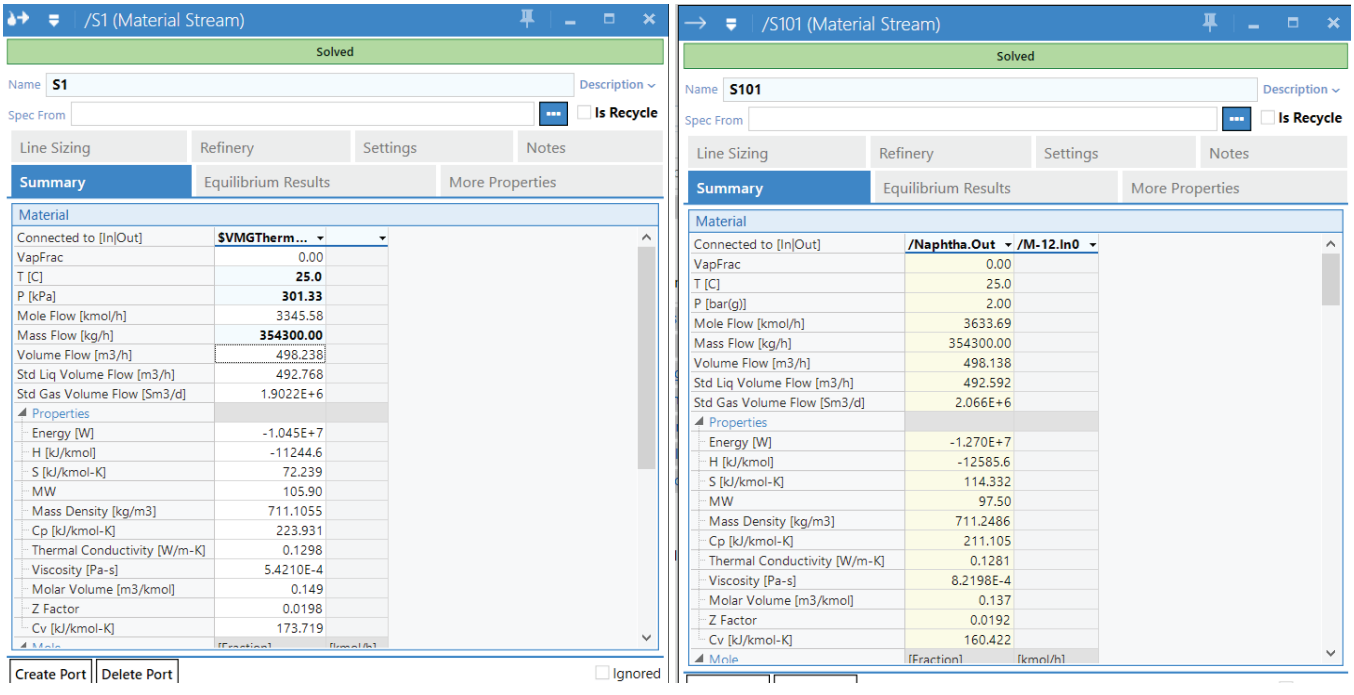

Figure 2 Stream properties comparison

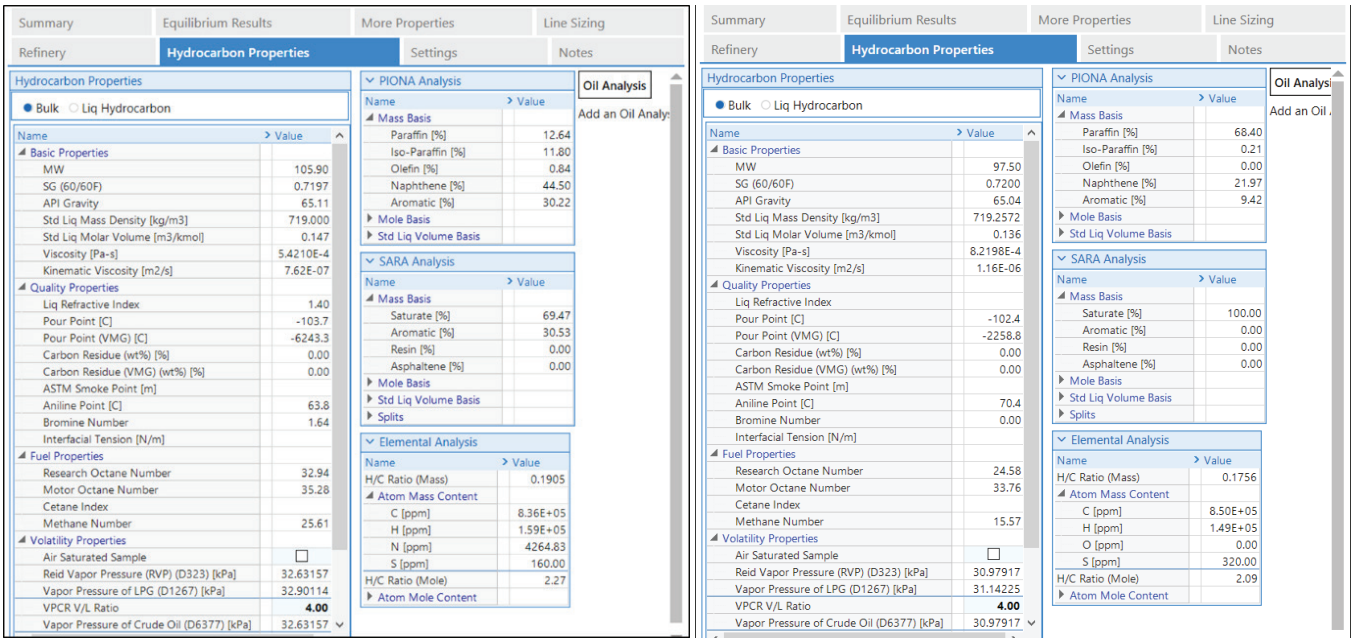

Figure 3 PIONA molecule distribution

components. The calculated PIONA distribution from PIONA characterisation has more Paraffin content as per Figure 3. This can lead to inaccurate product properties prediction such as RON, pout point, etc., affecting product quality.

CONCLUSION

This new PIONA characterisation approach provides a more accurate definition of refinery fluid properties that will support rigorous modelling of refinery equipment, especially the reactors (e.g., FCC, CCR, etc.) reaction path, and product distribution estimation depends heavily on the accurate PIONA distribution characterisation.

ACKNOWLEDGEMENT

I would like to acknowledge PETRONAS Group Technical Solutions and PETRONAS Refining and Petrochemical Corporation to access data and simulation software.

REFERENCES

iCON Symmetry 2020 User Manual, PETRONAS.