Characterization of Iraqi crude oil using Aspen Hysys

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Abstract. The economical value of crude oil is influenced by various chemical and physical properties, Therefore, enhancing the crude oil properties can be of great benefit for crude oil-exporting countries as Iraq. The process of enhancing crude oil properties can be carried out through the blending of different crude oils from different wells. In this research, we illustrate Iraqi crude oil enhancing through the blending of three different Iraqi oils, Nahran Umar Crude, Badra Crude, and West Qurna Crude. The blending process was carried out using a common industrially used simulator for the oil and gas field, Aspen HYSYS.

Keywords: Thermodynamic properties, crude oil, density, viscosity, specific heat, and thermal conductivity.

1 Introduction

Crude oil is a non-uniform admixture of different hydrocarbons, that in most cases would contain certain impurities including metals, chlorides, elemental nitrogen, nitrogen oxides, elemental sulfur, hydrogen sulfide, hydrogen oxides, and mercaptans. The presence of certain impurities would affect the oil quality. For example, crude oil can be classified as light, medium, or heavy crude according to its density which is directly influenced by the length and structure of the hydrocarbon chains, it may be also classified as sweet or sour based on sulfur content or classified as naphthenic, paraffinic or aromatic (Abdel-Raouf, 2012).

The API gravity of medium crude oils ranges from 22.3 to 31.1 above which the crude is classified as light crude otherwise it's considered heavy crude oil. The higher API gravity, the lower the sulfur content. Crude oil of sulfur content below 0.5% in weight is known as sweet oil otherwise is sour (Bennett,2016). Naphthenic, paraffinic, and aromatic nature can be estimated based on the Watson Characterization Factor (KW) with naphthenic oils in the range of 10 to 11, paraffinic in the range of 11 to 12.9 (Scherzer et al, 1996).

Taking into consideration that each refinery would have a unique design based on the feed specifications and produced petroleum products and that well production capacity and crude oil properties interface certain changes along well lifetime. Therefore, crude oil blending can be considered a must for certain refineries. Light crude distillation produces higher yields per unit mass of high-value products like gasoline compared to medium and heavy crudes consuming less energy in form of heat. On the other hand, transportation and storage costs of light crudes are relatively low which makes light oils more favorable for refineries (Speight, 2001). The purpose

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of crude oils blending is to obtain a new blend with certain properties to ease transportation, meet feed specifications of certain plants, making use of lower grade oils by mixing a small portion with high-grade oils, etc (Demirbas, 2017).

Enhancing crude oil properties through blending processes has been studied for many years. García and Urbina (2003) characterized sixteen crude oils from Eastern Venezuela in terms of wax content, hydrocarbons distribution, and other factors, to study those factor effects on the flowing properties of these crudes and their blends. Some blends of those crudes showed significant improvement in oil flow decreasing the wax crystallization tendency.

Li et al. (2006) investigated the blending process of Cabinda oil and Oman oil to obtain the optimum blending ratio that would form a suitable feedstock for a certain refining operation. They studied the distillation products' yields showing an optimal blending ratio of 7:3 for the Cabinda oil and Oman oil respectively. They also validated relationships between yields, viscosities, and surface tension.

Centeno et al. (2011) reported seventeen mixing rules that were used for the prediction of crude oil viscosity and its fractions. The mixing rules were examined and validated by comparing estimated values with experimental viscosities of various crudes of various API gravities. It was reported that only four of the tested rules showed the good ability of crude prediction (Chevron, Walther, Einstein, and Power-law), while no rule was able to calculate the viscosity of all the crudes successfully, A fifth rule (Chririnos) showed good accuracy for the prediction of distilled products such as naphtha.

Hou et al. (2015) established a model for crude oil optimization and properties prediction for Shanbei crude blending, which aims to improve the total yield of fractions and to reduce the viscosity of the blend. The model was used to predict the results of two different blends. Blends were later prepared and distilled to validate the model.

Hernández et al. (2019) investigated important mixing rules to estimate the viscosity of blended crude oils. Experimental viscosity of various binary and tertiary crude oil blends was tested in labs and used to validate the mixing model and determine its accuracy. They proved that the mixing rule with 4 interaction parameters has the highest ever efficiency compared to conventional mixing rules. Interaction parameters were obtained by statistical techniques and sensitivity analysis.

Naji et al. (2021) investigated the blending process of different Iraqi oils and its effect on obtained blend API gravity and sulfur content. They also simulated the fractionation process of different blends to predict atmospheric distillation products' yields and quality. The aim of the research. Characterization and analysis of the thermodynamic properties, including density, viscosity, specific heat, and thermal conductivity of Iraqi crude oils. this is of great importance in the stage that comes after the extraction process, which is dealing with these oils in transportation and storage operations.

2 The Aim of the Research

In this research, we aim to characterize and analyse thermo-mechanical properties of three different Iraqi crude oils and their blends, including density, viscosity, specific heat, and thermal conductivity. The importance of such properties becomes clear during the early design stages of refineries.

3 Blending Process Simulation

The simulation process was carried out using two different software's "Aspen HYSYS ®" and "Aspen Plus ®" provided by Aspen Tech Inc. Both simulators have widely proved their ability to solve complex industrial models that handle material balance calculations, heat balance and heat transfer calculations, vapor-liquid equilibrium (VLE) calculations, hydraulics calculations. The two simulators contain built-in thermodynamic models known as "Fluid Packages''.

A. Fluid Package Selection

The selection of an adequate fluid package depends mainly on the process itself as well as the chemical components we would deal with, with Aspen Tech providing a "method assistant" the fluid package of "Peng-Robison (PR)" was selected.

According to the Aspen Tech user guide (Aspen Tech, 2000), Peng-Robinson (PR) model is the most used thermodynamic model for (VLE) calculations in Oil & Gas industries, especially when dealing with hydrocarbons at temperatures above -271 °C, below 900 °C, and pressures below 100,000 kPa.

B. Crude Oils Defining

The three crudes were imported to Aspen HYSYS ® and Aspen Plus ® in form of crude assays. Assay data type was selected as "True Boiling Point (TBP) weight basis" due to available crudes lab data. Imported assays included light ends (C1:C5) analysis, TBP curves, molecular weight curves, kinematic viscosity curves at 20 °C and 100 °C, density curves, sulfur content curves, and bulk properties like API gravities, Watson factors, and viscosities. Table 1 represents a classification summary of each crude oil.

Table 1. Crude Oils classification summary.

Crude Properties	Crude (1)	Crude (2)	Crude (3)
API gravity	42.9	35.5	22.8
Watson Factor	12	11.9	11.6
Sulphur Content wt%	1.19	2.31	4.13
Classification	Light, Paraffinic, Sour	Light, Paraffinic, Sour	Medium, Paraffinic, Sour

4 Results and Discussion

Data obtained through Aspen HYSYS ® was re-arranged and visualized using MATLAB ® software.

4.1 Heat Capacity

Specific heat capacity for a certain substance represents the amount of supplied energy required to increase the temperature of this substance one degree Celsius, and thus for a crude blend of high specific heat. Capacity would require much energy for the refining process.

i. Mass Heat Capacity

Results showed that increment blending percentage of crude (3) would significantly decrease the overall blend mass heat capacity while increasing the percentage of crude (2) would have no significant effect. This is due to the small difference between crude (1) and crude (2) mass heat capacities, 1.846 and 1.847 kJ/kg. respectively, and the low mass heat capacity of crude (3), 1.472 kJ/kg., compared to other crudes. Fig 1**.** illustrates the variation of mass heat capacity for different blending ratios.

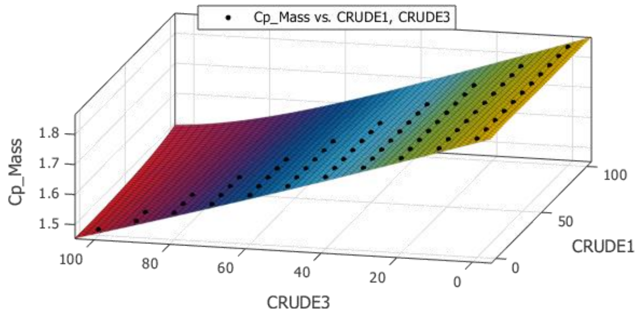

Fig 1. Variation of Mass Heat Capacity for Different Blending Ratios.

ii. Molar Heat Capacity

Molar heat capacities of crude (1), crude (2), and crude (3) were estimated as 293.6, 341.1, and 693.8 kJ/kmol.°C respectively. Unlike the variation scheme of mass heat capacity, increasing the blending percentage of crude (3) increases the molar heat capacity of the overall blend severely. On the other hand, increasing the blending percentage of crude (2) has a significant effect in increasing the blend molar heat capacity. Fig 2. shows the variation of molar heat capacity for tertiary blending.

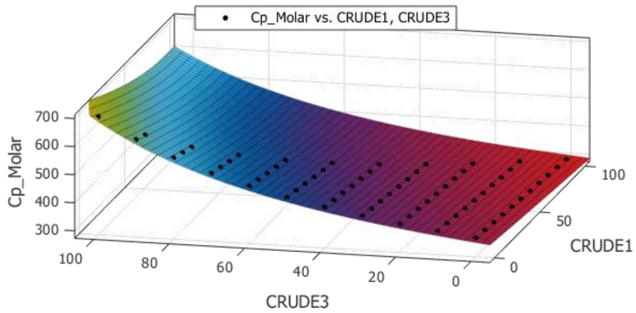

Fig 2. Variation of Molar Heat Capacity for Different Blending Ratios.

The irreconcilable behaviour of mass and molar heat capacities variation for tertiary blending is supposed to be due to the significant difference in molar mass of each blend which was reported to be 159, 184.7, and 471.2 kg/kmol for crude (1), crude (2) and crude (3) respectively.

4.2 Latent Heat of Vaporization

Standard heat of vaporization of various blending scenarios was analysed. The importance of such thermal property is summarized in estimating energy demands of atmospheric distillation units' re-boilers side by side with heat capacity. Results showed that increasing the blending percentage of crude (3) would lead to a severe increase in heat of vaporization of the obtained blend and thus the re-boiler duty. While increasing crude (2) blending percentage would increase the blend heat of vaporization but less sharply.
Specific heats of vaporization were estimated as 173.7, 230.6, and 453.1 MJ/kmol for crude (1), crude (2), and crude (3) respectively. Fig 3. shows the variation of molar heat of vaporization for tertiary blending.

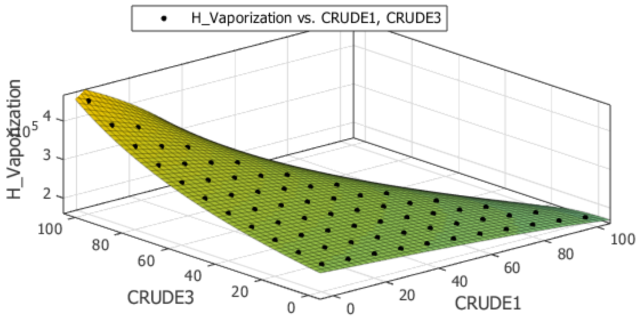

Fig 3. Variation of Heat of Vaporization for Different Blending Ratios.

4.3 Thermal Conductivity

The importance of thermal conductivity of the obtained blend is an accurate estimation of heat transfer coefficients for the refinery pre-heaters and boilers. Thus, variation of thermal conductivity of the blend was studied for various blending ratios. Fig 4. shows the variation of thermal conductivity in W/m.k for tertiary blending.

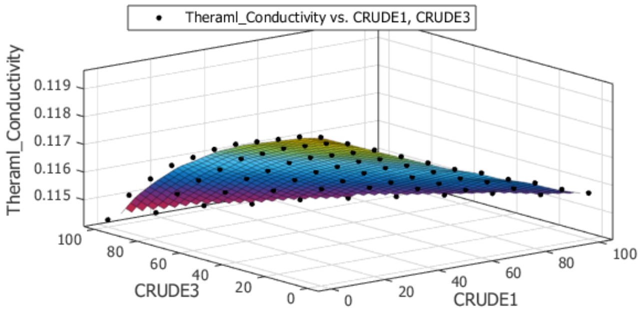

Fig 4. Variation of Thermal Conductivity for Different Blending Ratios.

4.4 Heat Capacity

Viscosity is one of the most used properties in calculations related to momentum transfer, fluid flow, and heat transfer. Thus, estimation of blend viscosity for various blending ratios is of great importance. Results collected from the Aspen HYSYS case study were analysed and plotted in Figs 5 & 6. Since viscosity is a temperature-dependent property, it's not easy to compute all viscosity variation possibilities. In this case, we study the viscosity variation due to variation of blending ratios at a constant temperature of 60 °F.

Results showed that increasing the percentage of crude (3) in the blend would increase both dynamic and kinematic viscosities of the blend severely. While increasing crude (2) percentage in the blend would have no significant effect on neither dynamic nor kinematic viscosities of the blend for low percentages of crude (3). For high percentages of crude (1), neither increasing crude (2) nor crude (3) percentages would have a significant effect on dynamic or kinematic viscosities.

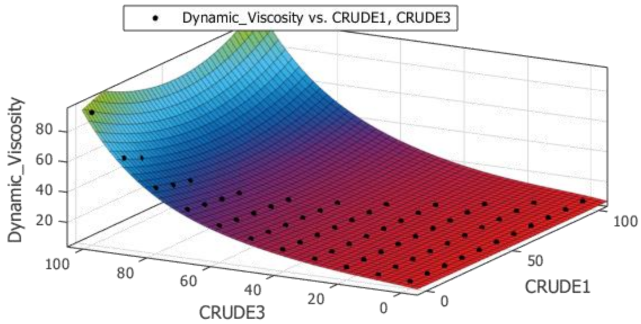

Fig 5. Variation of Dynamic Viscosity for Different Blending Ratios.

4.5 Adiabatic Index

The adiabatic index, also known as the isentropic expansion factor, is the ratio of heat capacity at constant pressure to heat capacity at constant volume, it's important in the evaluation of adiabatic expansion and compression of fluids, represented in fluid behaviour within distillation columns in this case.

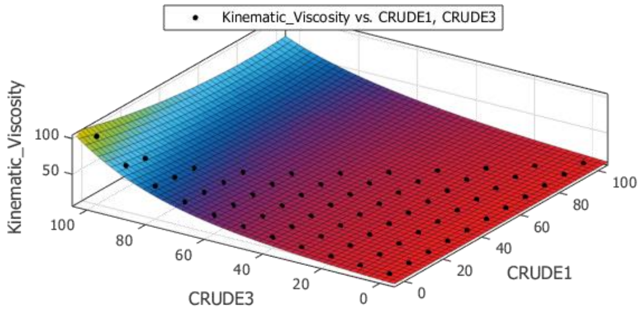

Fig 6. Variation of Kinematic Viscosity for Different Blending Ratios.

The adiabatic index for the blend was studied for various blending ratios and reported in Fig 7. Results showed that increasing the percentage of crude (3) in the blend would have a dramatic decrease in the adiabatic index of the blend while increasing crude (2) percentage has a small influence in decreasing the adiabatic index.

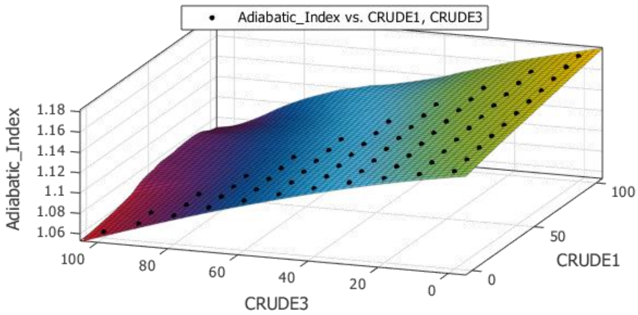

Fig 7. Variation of Adiabatic Index for Different Blending Ratios.

5 Conclusion

Depending on simulation results we conclude that the blending process of different grade crude oils can significantly enhance certain thermo-mechanical properties. With small changes in blend ratio, certain properties would change significantly and thus performing simulation studies for rating purposes of already installed petroleum refineries can be of great importance to prepare the optimum feed blend.

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