Expansion of the p:IGI+ SARA Property Model

by Andrew Green

The goal in creating the new p:IGI+ property model was to provide a comprehensive and meaningful property model which provides our software users with the ability to correctly record their data and associated meta-data while also providing appropriate means for intelligent interpretation given appropriate knowledge of how the data were acquired.

One area of geochemical analysis that has experienced a complete overhaul in the p:IGI+ data model is the quantification of the proportions of the different bulk fractions of oil or extracted bitumen - commonly referred to as SARA analysis (Saturated hydrocarbons, Aromatic hydrocarbons, Resins (or polar NSO compounds) and Asphaltenes). As with many geochemical analytical techniques there are several possible approaches to fractionating an extracted bitumen or oil depending on the end goal. Three common fractionation methods employed in the industry are:

- **Column Chromatography (CC):** The separation of a whole oil/extract sample ahead of further analysis of either a Saturated hydrocarbon, Aromatic hydrocarbon, Resins or Asphaltene fraction through the relative differences in molecular affinity between the mobile and stationary phases
    - **Thin Layer Chromatography (TLC):** follows similar separation principles to CC but is mainly used for separating smaller samples
- **Iatroscan (FID):** A cost effective bulk composition analysis approach conducted on whole oil/extract samples, but the separated compound fractions are destroyed during analysis. The Iatroscan was designed as an automated form of TLC
- **Medium or High Pressure Liquid Chromatography (MPLC or HPLC):** The most commonly employed separation method used in service laboratories ahead of further analysis of either a Saturated hydrocarbon, Aromatic hydrocarbon, or Resins fraction. Separation normally uses a previously deasphaltened oil/extract sample

Entering SARA data into p:IGI-3 (Extract analysis page) requires the user to give careful consideration to sample type and fractionation method utilised (Fig.1) as many of the property columns hold multiple definitions (e.g. Asph: conducting MPLC involves prior determination of precipitated wt% Asph, while conducting Iatroscan FID records the fractionated wt% Asph). Table 1 provides a summary of how p:IGI-3 would normally be populated giving consideration to sample type and fractionation method.

p:IGI-3 SARA Property Model present on (Extract Analysis Page)						
			Extract Fractionation Method & Result			
Cell No#	Prop	Unit	CC/TLC	MPLC/HPLC	Iatroscan FID	Comment
<84>	Smpl Wt	g	Y	Y	Y	Rock Weight
<85>	WtExtr/Oil	g	Y	Y	Y	Extract Weight
<86>	ExtYield	mg/g	Y	Y	Y	Yield of Extract
<457>	Loss topping	Wt%	N/A	N/A	N/A	Loss on topping at 2Y0°C Oil Only
<456>	Extract Method		Y	Y	Y	Important piece of Metadata
<87>	Sats	Wt%	Y	Y	Y	
<88>	Arom	Wt%	Y	Y	Y	
<89>	NSO	Wt%	Y	Y	Y	
<90>	Asph	Wt%	N/A	Y	Y	Asphalt MPLC=Precip / Iatroscan=FID
<91>	Other	Wt%	Y	N/A	N/A	Asphalt is present in other fraction
<92>	Difference	Wt%	Y	Y	Y	%Loss on fractionation
<93>	CNE	mgExtr/gTOC	Y	Y	Y	
<94>	CNH	mgHC/gTOC	Y	Y	Y	
<95>	Sats/Arom	a/b	Y	Y	Y	

			Oil Fractionation Method & Result			
Cell No#	Prop	Unit	CC/TLC	MPLC/HPLC	Iatroscan FID	Comment
<84>	Smpl Wt	g	Y	Y	Y	Untopped Oil Weight
<85>	WtExtr/Oil	g	Y	Y	Y	Topped Oil Weight
<86>	ExtYield	mg/g	Y	Y	Y	Yield of Topped oil
<457>	Loss topping	Wt%	Y	Y	Y	Loss on topping at 2Y0°C Oil Only
<456>	Extract Method		Y	Y	Y	Important piece of Metadata
<87>	Sats	Wt%	Y	Y	Y	
<88>	Arom	Wt%	Y	Y	Y	
<89>	NSO	Wt%	Y	Y	Y	
<90>	Asph	Wt%	N/A	Y	Y	Asphalt MPLC=Precip / Iatroscan=FID
<91>	Other	Wt%	Y	N/A	N/A	Asphalt is present in other fraction
<92>	Difference	Wt%	Y	Y	Y	%Loss on fractionation
<93>	CNE	mgExtr/gTOC	N/A	N/A	N/A	No TOC available for Fluids
<94>	CNH	mgHC/gTOC	N/A	N/A	N/A	No TOC available for Fluids
<95>	Sats/Arom	a/b	Y	Y	Y	

Table 1: Summary of how the SARA data would normally be populated in the p:IGI-3 property model. The user would have to give careful consideration to sample type and fraction method utilised.

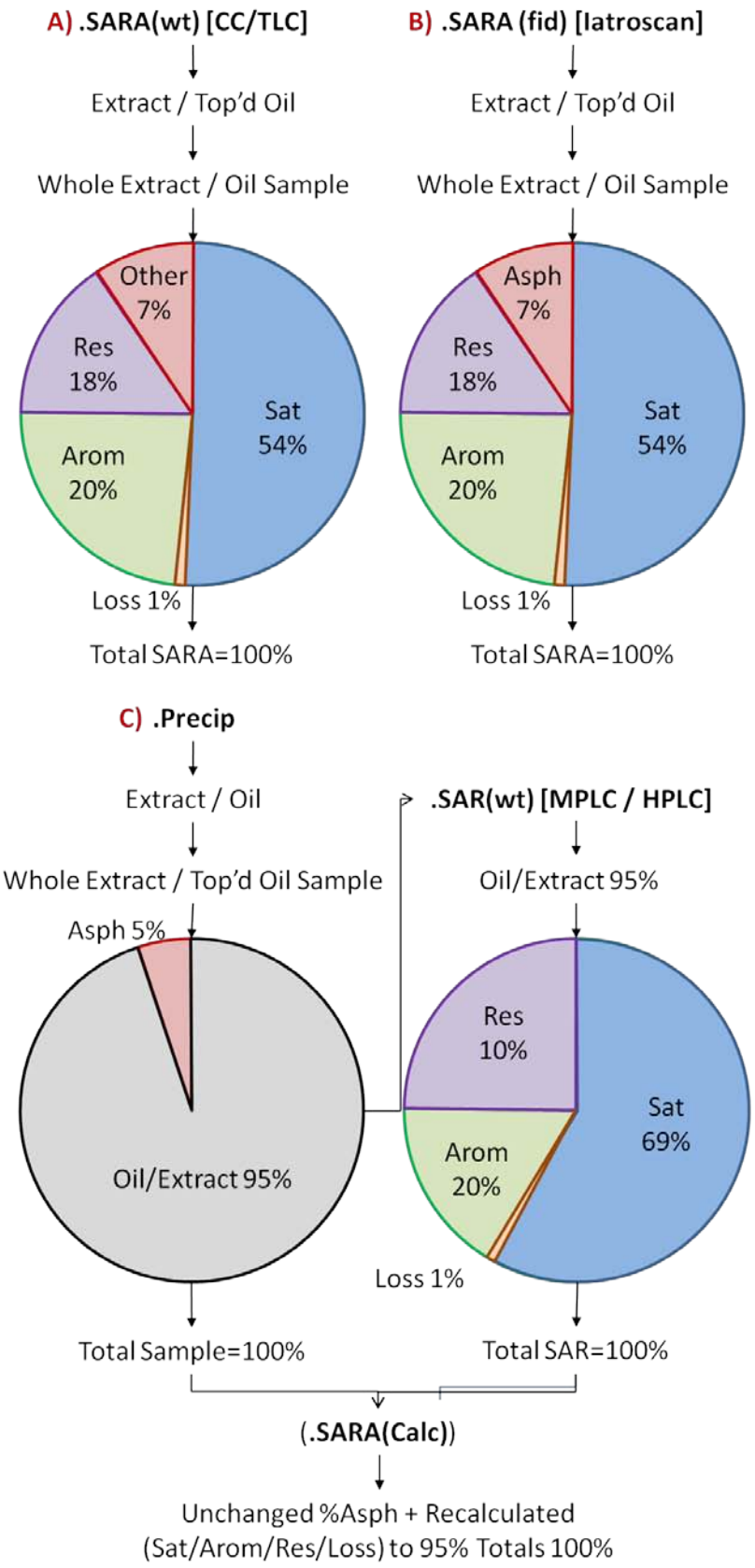

Figure 1. Summary of the different fraction methods available along with a guide to the workflow associated with each method. Example values represent weight fractions (%wt).

p:IGI+ property naming components:

Property Name[indicator].Analysis Group (Description) (Unit, Ratio Format)

Format presented everywhere a property selection is required:

Property Name.Analysis Group (Description)

Format presented on created graphs:

Property Name[indicator].Analysis Group (Unit, Ratio Format)

Figure 2. The p:IGI+ property model naming convention and display format used. Not all naming components are necessary for certain properties. For example a property Indicator is only assigned either a molecular or gas property where multiple data forms are reported [height, area, concentration height/area, unknown].

The p:IGI+ property model has been comprehensively developed using a cleaner naming convention (Fig. 2) providing a clearer differentiation of analytical work flow and data source. Figure 3 displays the relevant parts of the new p:IGI+ property model along with the given *default* linkages (these are manually editable during import) when importing p:IGI-3 files into p:IGI+. At present the default linking makes the following assumptions:

1. All samples have been extracted
2. All samples have been analysed using MPLC of HPLC
3. All asphaltene data originate from precipitation methods

The main analysis groups relating to this area of the property model in p:IGI+ are:

- **SAR(wt):** this is appropriate for MPLC/HPLC data obtained after asphaltene precipitation.
- **SARA(calc):** this will be auto-populated from raw SAR(wt) data and precipitation information in most cases, but can be used for values taken from tables where renormalisation has been already applied.
- **SARA(wt)**: this is appropriate for CC / TLC data which includes a measurement of asphaltene fraction directly, recorded in the %other property, since these methods cannot directly measure the asphaltene fraction weight alone.
- **SARA(fid):** this is appropriate for FID (Iatroscan) data.

The choice of which analysis group to use will not always be clear given the metadata accompanying the data. In the situation of an unknown origin or for the data reported with no %Asph value IGI would recommend linking data the SARA(calc) analysis group. This does assume the reported fractions have been renormalized with the consideration for an ashpaltene fraction which could be seen as a negative. However positively it assumes the most commonly analytical approach has been used to produce the data and ensures the data can be utilised in an interpretative context through the **.Any** analysis group.

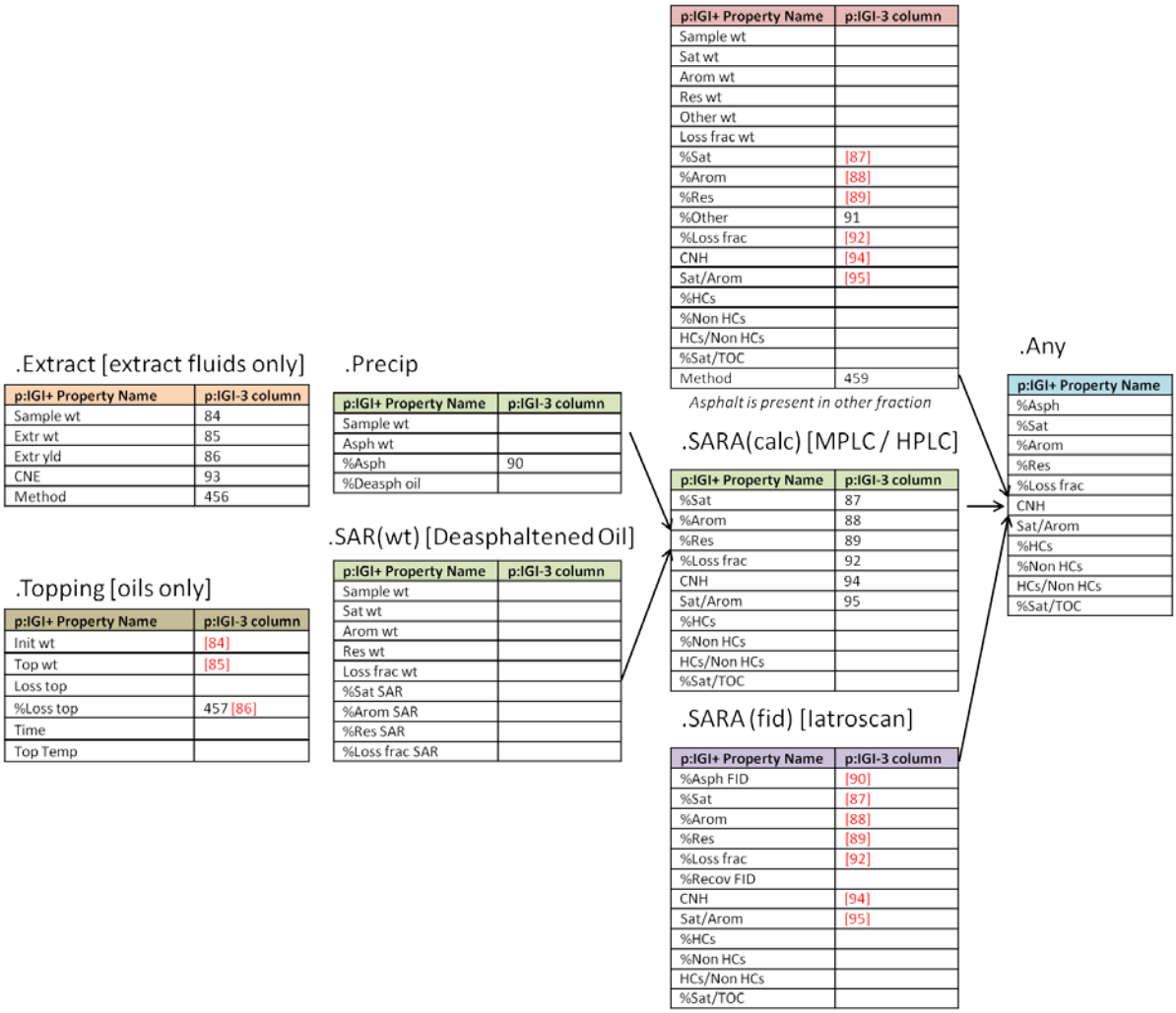

Figure 3. Summary of how the SARA property model has been organised in p:IGI+. Accompanying the conceptual layout of the SARA property model are both the p:IGI-3 default property mappings (black number showing the p:IGI-3 column No.) and additional manual remapping options for import of alternate sample type or analytical methods other than the assumed defaults (red number showing p:IGI-3 column No.). For interpretation applications (e.g. palettes, graph axes or SampleSets) the respective properties from the .Any analysis group should be chosen, if an overview of all data is desired.

With p:IGI+ SARA data now stored in different property columns based on the preparative and analytical method used (Fig. 3), the interpretative application of this property model is maintained through the introduction of an **.Any** analysis group and associated properties. **.Any** properties recombine data into unified property columns for the purposes of graphical data display (*i.e.* showing all samples with any appropriate data, irrespective of the method used).