ADIOS DB Data Model: version 0.11.0

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Feb, 2021

Introduction

This document lays out the data model for an oil record in the ADIOS database. The goal of this data model is to be able to accommodate a wide variety of data that is associated with a particular product in the database, while providing enough structure that the data can be worked with in standard ways.

Along with the data model, this document provides examples of storing that data in the JSON file format -- the format used by NOAA's ADIOS-DB for storage and data interchange.

But data in any format that provides the information described in this document should be importable into the database.

Table of Contents:

Building Blocks

This data model is based on a few concepts that can be nested arbitrarily: “Structures”, with a fixed number of defined elements (e.g SARA analysis) and “Lists”, collections of similar items (either structures or lists themselves) (e.g. Compounds). Items in a list will usually have a name in order to keep the items apart.

Every structure in the data model can have an optional “notes” field for arbitrary notes about that specific data.

For more detail on particular structures used, see: Definitions of Data Types

Oil Record

ID

Unique identifier for the record: this would generally be assigned by the database, so it is not technically part of the data for the record.
Type: text
Example: “AD000003"

Record Metadata

Metadata is a structure of attributes which describe the oil record.

Name

A human-readable name for the record -- ideally unique

Type: text
Example: "Access West Winter Blend"

Additional Identifiers

A list of other names, etc that may be applied to this record, e.g. the region, field name, etc. Important is that these names are specific to the particular record -- not generic descriptions. E.g. you might put “Macondo” and “MC 252” for oil from the Deepwater Horizon incident. But “diesel” is not specific to that record -- “diesel” would be appropriate for a label, however.

Source Identifier

Identifier used by the source of the data: the lab that did the analysis, etc. This is intended to be a short ID, not a description. The human-readable names should be in the name or additional identifier.

Type: text
Example: “HOOPS16F"

Reference

The full bibliographic reference, it has two components:

Year: year of publication
Type: number
Example: 2013
Reference: The complete reference

Type: text
Example: “Hollebone B. "Physical Properties and Behaviour Measurements of Alaskan North Slope [2013] Crude Oil", Environment Canada, Ottawa, Ontario, Canada, May 2013”

Sample Date:

Date the sample was taken from the source, or received by the lab.

Type: ISO 8601 text string (https://en.wikipedia.org/wiki/ISO_8601)
Example: “2020-03-19”

Location:

Location of source of oil (well, etc)

Type: text
Example: "Alberta, Canada"

Location Coordinates:

Georeferenced location of source of oil (well, etc). This can be a single point or a simple polygon delineating a region.

Type: one point lat-lon coordinates (Decimal degrees, WGS84):
Example: 28.324 , -76.521
or:
Type: Polygon: ordered list of multiple points’ lat-lon coordinates (Decimal degrees, WGS84):
Example: [(88.671327, 29.111853),(88.512073, 29.155960),(88.434388, 29.033772),(88.554800, 28.891036),(88.706286, -28.982817)]

Product Type:

General type of product, see: Product Types

Type: text, one of: defined list from: Product Type
Example: “Bitumen Blend”

Labels:

Assorted “tags” you may want to apply to the data (see section: Labels for the labels used by NOAA). THe primary goal is to have these be searchable. If someone Is looking for “fuel oil #2”, they should find all the number 2 fuel oils.

While a given record is one and only one Product Type, which defines what the product *is*, a record can have any number of labels, which are more or less what a product might be “called”, One of the reasons labels are useful is that petroleum products have many overlapping naming

and categorizing systems.e.g. a Diesel Fuel *is* a Distillate Fuel Oil, it can be *called* “diesel” or “number 2 fuel oil”. These are intended to be more generic than additional identifiers -- it is expected that a lot of records will have any given label.

Type: List of short text strings.
Example: [“Number 2 Fuel Oil”, “Light Refined Product”]

Comments:

Any additional information about the record that is not captured in the fixed fields.

Type: Free form text.
Example: “Sample Collected in the field by Patrick Star during the M/V Sponge Bob incident”

API Gravity

The API Gravity of the product. API is used primarily for reference, searching, etc. It should match the density at 15C. API is a particular unit for density at 60F (Almost 15C, but not quite). It should be computed from the density measurement, and only used for reference -- the included density data should be used for modeling, etc.

Type: number
Example: 36.2

Subsamples

Subsamples is a list of one of more individual samples that have been analysed. The first one in the list should be the “fresh” oil, as it first arrived at the lab. Other sub samples might be weathered, or distillation cuts, or otherwise processed before analysis.

Each Sample is a structure with metadata and data on samples that were derived from a single original oil sample.

Name:

The name given to this sample

Type: text
Example: Fraction left after Rotovap to 25% mass loss

Short Name:

An abbreviated form of the name that can be displayed easily

Type: text
Example: 25% weathered

Description:

This can be any text that describes the sub sample

Type: text

Example: “Sample weathered to 24% mass loss with a rotovap ...”

Sample ID:

An ID for the sub sample: each lab might have its own system for identifying their subsamples

Type: text

Example: “2234.1.3.1”

Evaporated fraction:

Some oil samples are evaporated artificially and this is the mass from loss in that process

Type: fraction: between zero and one, or percent, etc.

Example: 24%

Boiling Point Range:

Some oil samples are fractions collected through fractional distillation and are characterized by a boiling point range.

Type: pair of temperatures

Example: (160F to 330F)

Compounds

Compounds is a list of concentration measurements for zero or more individual compounds. Each item in the list has a standard structure with a name, method, measurement, and chemical groups:

An individual compound has the following elements:

Name: The name of the compound

Type: text

Example: "1-Methyl-2-Isopropylbenzene"

Method: The laboratory method used for the measurement

Type: text

Example: "ASTM D5002"

Groups: Any groupings that may be relevant to the compound

Type: List of zero or more groups, as text.

Example: ["Phenanthrenes", "PAH 50”]

Measurement: The actual measurement of the compound
Type: Measurement (see below)
Example: 3.4 ppm (mass fraction)

JSON Example:

Bulk Composition

Bulk Composition is a list of zero or more groupings of chemicals as opposed to individual compounds. Examples are in the Common Data section below. Like the Compounds list, each object in the list has the same structure including the following elements:

Name: Chemical Category Name
Type: text
Example: "Wax Content"
Method: The laboratory method used for the measurement
Type: text
Example: "ESTS 12.11/2.0/M"
Measurement: The actual measurement of the compound
Type: Measurement (see below)
Example: 4.0% (mass fraction)

Physical Properties

Physical Properties is a structure with these specific elements. Each element may have a unique structure required to fit its needs.

Density: The density of the oil. Density varies with temperature, so it is usually measured at multiple temperatures; so this is a list of multiple individual density measurements at different temperatures, each defined as so:
Method: The method used
Type: text
Example:”ANSI XXXX”
Density: The density measured
Type: Measurement
Example: 0.87 g/cm^3
Reference Temp: The temperature the density was measured at
Type: Measurement
Example: 15C

Kinematic Viscosity: The kinematic viscosity of the sample. Viscosity varies with temperature, and sometimes shear rate; so Kinematic Viscosity is a list of individual measurements, at a specified temperature and shear rate, defined as so:
Method: The method used
Type: text

Example:”ANSI XXXX”

Kinematic Viscosity: The measured viscosity

Type: Measurement

Example: 5,000 centiStoke

Reference Temp: The temperature the density was measured at

Type: Measurement

Example: 15C

Shear Rate: The shear rate of the measurement

Type: Measurement

Example: 100 1/s

Dynamic Viscosity: The dynamic viscosity of the sample. A list of individual measurements, the same as kinematic viscosity.

Pour Point: The temperature below which the liquid loses its flow characteristics. It is a single structure with a method and a measurement.

Method: The method used

Type: text

Example:”ASTM D97”

Pour Point: The pour point value

Type: Measurement (temperature)

Example: -5 C

Flash Point: the lowest temperature at which the oil’s vapors ignite if given an ignition source. It is a single structure with a method and a measurement.

Method: The method used

Type: text

Example:”ASTM D7094”

Flash Point: The flash point value

Type: Measurement (temperature)

Example: 13 C

Interfacial Tension: the tendency of liquid surfaces to shrink into the minimum surface area possible. The interfacial tension of oil can be different depending on the other liquid, and is different at different temperatures. Thus there can be three entries:

Oil-Water

Oil-Seawater

Oil-Air

Each entry is a list of multiple measurements at different temperatures:

Method: The method used

Type: text

Example:”ESTS 12.12/x.x/M”

Interfacial Tension: The tension measured
Type: Measurement
Example: 1.13 dynes/cm
Reference Temp: The temperature the density was measured at
Type: Measurement
Example: 0C

Industry Properties

Properties of the oil that are often used by the oil industry. Examples are in the Common Data section below.

These are stored in a list of zero or more items. Each item has the following elements:

Name: The name of the property, test, etc.
Type: text
Example: “Cetane Index”
Method: The method used
Type: text
Example: “D4737”
Measurement: The measured value
Type: measurement
Example: 36.2 (unitless)

Distillation Data

Distillation data is provided as a set of values for vapor temperature and fraction distilled. It contains the following data:

Type: Type of distillation: either mass fraction or volume fraction
Type: text “mass” or “volume”
Example: “volume”
Method: The method used
Type: text
Example: “Simulated Distillation: ASTM XXXX”
Mass Fraction Included: What fraction of the total oil is included in the distillation cuts.
Type: measurement: mass fraction
Example: 80% mass fraction
Note: Empty or None if unknown.
Distillation Cuts: The actual distillation cuts
Type: list of pairs of fraction and vapor_temp, with units
Example: 5% at 105.7F, 10% at 175.7F, 20% at 267.2F

Each distillation cut has the following structure:

Fraction: The mass or volume fraction of the cut

Type: measurement

Example: 13%

Vapor Temperature: The vapor temperature of this cut

Type: measurement

Example: 105.7F

End Point: The final temp of the distillation

Type: measurement

Example: 945F

JSON Example

Environmental Behavior

Environmental Behavior is a structured list of data pertaining to tests performed to determine the behavior of the oil in the environment.

Emulsion Data:

Emulsion Data is a list of emulsion data. It can contain a variety of measurements of emulsion properties

Each element in the list has the following attributes:

Age:

Type: Measurement

Example: One week after formation

Reference Temperature:

Type: Measurement

Example: One week after formation

Method

Type: text

Example:

Water Content:

Type: Measurement

Example:

Visual Stability:

Type: text

Example: “not formed”

Complex Modulus:

Type: Measurement

Example:

Storage Modulus:

Type: Measurement
Example:

Loss Modulus:
Type: Measurement
Example:

Tan Delta:
Type: Measurement
Example:

Complex viscosity:
Type: Measurement
Example:

ESTS Evaporation Test:

Evaporation Test is a structure with ESTS's evaporation equation for the oil sample

Method:
Type: text

Form of equation:
Type: text
Example:

Parameter A:
Type: number

Parameter B:
Type: number

Parameter C:
Type: number

Chemical Dispersibility Test: Chemical Dispersibility Test is the results of testing dispersibility with various chemical dispersants. It is a list of structures, one for each type of dispersant tested.

Name of Dispersant:
Type: text
Example: Corexit 9500

Method:
Type: text
Example: ASTM F2059

Measurement:
Type: measurement
Example: 10% with a standard deviation of 2.0 and 6 replicates.

JSON Example

Adhesion: Adhesion is a structure with the following elements:

Method:

Type: text
Example: Needle Adhesion Test (ESTS Method 12.12/x.x/M)

Measurement:
Type: Measurement
Example: 40 g/cm^2 with a standard deviation of 9.9 and 5 replicates

Reference Temperature:
Type: measurement
Example: room temperature.

Fractionations

There are various ways to break down a petroleum product into groupings of similar type. What these all have in common is that the total of all the parts should add up to 100% of the oil. We currently have three types of fractionations: SARA, CCME, and ESTS Hydrocarbon fractions.

SARA

SARA Analysis is the dividing of oils into four categories: Saturates, Aromatics, Asphaltenes and Resins. The SARA group will have those four attributes, and a method:

Method: The laboratory method used for the SARA analysis
Type: text.
Example: "12.11/1.0/M"

Saturates: The saturate fraction
Type: Measurement
Example: 38% (mass fraction)

Aromatics: The aromatic fraction
Type: Measurement
Example: 31% (mass fraction)

Resins: The resin fraction
Type: Measurement
Example: 16% (mass fraction)

Asphaltenes: The asphaltene fraction
Type: Measurement
Example: 15% (mass fraction)

JSON Example

CCME

CCME refers to a method for measuring contamination of environmental media which was originally published by the Canadian Council of Ministers of the Environment and is used for soil remediation regulations in Canada. More information can be found at the following link: https://www.ccme.ca/en/resources/contaminated_site_management/phc_cws_in_soil.html

It includes four “fractions”:

CCME F1: CCME Fraction # 1
Type: mass fraction
Example: 16 mg/kg

CCME F2: CCME Fraction # 2
Type: mass fraction
Example: 50 mg/kg

CCME F3: CCME Fraction # 3
Type: mass fraction
Example: 193 mg/kg

CCME F4: CCME Fraction # 4
Type: mass fraction
Example: 40 mg/kg

JSON Example

ESTS Hydrocarbon Fractions:

Environment Canada ESTS lab has developed an internal method to essentially measure pseudocomponents of an oil.

Method:

This method is similar to a simulated distillation, but it is not a standard method. First, the bulk oil is run through a chromatographic column where a saturate fraction and an aromatic fraction are isolated using various solvents with different polarities. Once the fractions have been isolated, they along with a mixed sample (reported as GC-TPH) are run through a GC-FID along with a reference sample which contains the named compounds (a series of straight-chain alkanes). The chromatograms of the saturate and aromatic oil fractions are then “cut” on the computer by integrating the areas between the peaks of the reference compounds. The resulting simulated concentration data are what is reported in the spreadsheet.

Saturates:

List of the saturates. Each element of the list has:
Name: The name of the grouping
Type: measurement (unit type: mass fraction)
Example: 16 mg/g n-C10 to n-C12

Aromatics:

List of the aromatics. Each element of the list has:
Name: The name of the grouping

Type: measurement (unit type: mass fraction)
Example: 13 mg/g n-C16 to n-C20

GC-TPH:

List of the total TPH. Each element of the list has:

Name: The name of the grouping
Type: measurement (unit type: mass fraction)
Example: 40 mg/g n-C34+

JSON Example

Definitions of Data Types

A limited number of structures and data types are used in the database.

Measurement

Much of the data in a record is a measurement of some sort. The measurement is designed to be flexible, accommodating single values, a range of values, and specification of replicates and a standard deviation, if applicable. An individual measurement contains the following information:

Value, Unit, and Unit type are required.
Replicates and Standard Deviation are optional.

Value: to accommodate a range of values, a measurement can have either a single value or a minimum and maximum value. If there is a minimum value but no maximum value, then it is interpreted as greater than or equal to the minimum. If there is a maximum and no minimum, then it is interpreted as less than or equal to the maximum. Note that values should contain only the number of digits appropriate to the precision of the measurement.

All items:

Single Value: The value of the measurement.
Type: number or None (if not defined, min and/or max must be defined)
Example: 3.451

Minimum Value: The minimum value if there is a range of values
Type: number or None (if specified, Value must not be defined)
Example: 2.4

Maximum Value: The maximum value if there is a range of values

Type: number or None (If specified, Value must not be defined)
Example: 5.3

Unit: The units the value is in.
Type: text
Example: “ppm”

Unit Type: The type of the unit -- usually the dimensionality
Type: text
Example: “length”, “mass”

Replicates: Number of replicates taken, if applicable
Type: integer.
Example: 3

Standard Deviation: Standard deviation of replicates, if applicable (in same units as the value!)
Type: number
Example: 2.31

Replicates and Standard Deviation can be omitted if there was only one replicate.

Units

Knowing the units of a value is critical to understanding and using that data. In this data model, every value should be accompanied by a well specified unit. Each unit must also have a defined “unit type” -- that is, what physical quantity that unit represents. Many units are clear and unambiguous in this regard: meter is a length, gram is a mass, etc. But many units can be ambiguous from just the name: “oz” could be a weight or a volume (fluid oz). In order to make sure there is no ambiguity, the unit type should be specified in all cases.

Practicalities

For the most part, SI or CGS (centimeter, gram, second) units are prefered. However, many measurements in the petroleum industry have commonly used units that do not conform to SI. Any properly specified unit is acceptable, so that units familiar to the user can be used.

Concentrations

Concentration is technically “unitless”, that is: a simple fractional number: percent, or parts per million, etc. However, these fractional values can have different physical meanings. In order to make sure there is no ambiguity, the Unit Type should be specified to make it clear: “Mass Fraction” or “Volume Fraction” or “Concentration in Water”. This will allow conversion between,

e.g. g/kg and ppm without ambiguity. It will also reasonably disallow conversion between, e.g. g/kg and mL/L.

Compound Units

Many values are well defined “compound units”: units that are clear combinations of base physical units. For example density is in units of mass per volume. While this is clearly describable in terms of base physical units, in the petroleum (and spill response) industry, there are many units that do not conform to the usual rules, such as API gravity. Thus, in this data model, compound unit types are specified as unique types, such as “density” and “kinematic viscosity”. However, it is still preferred that “proper” units be used for these values, such as $kg \cdot m^{-1} \cdot s^{-1}$ instead of Saybolt FUROL seconds for kinematic viscosity.

Allowed units

The unit types and units allowed are those specified in the unit data in the NOAA Unit Converter for OIl Spills (NUCOS):

https://github.com/NOAA-ORR-ERD/PyNUCOS/blob/master/NUCOS_unit_list.rst

[NOTE: This should be copied into this document when we are ready to publish it.]

Product Types

The Product Type is a broad identifier of the general class of product. It can be interpreted by users to, at a quick glance, know what the product is. It can also potentially be used by models to select appropriate algorithms to apply to the product. Essentially, the product type defines what the product “is”.

The Product Type must be one of a set list, outlined below. Every record should belong to one and only one product type. If a record is for a product that does not fit into any product type, it can be typed as “other”. If it is unknown what the product type is, it should be given no product type. That is, other means: “Not one of the existing product types”, rather than “not sure what this is” Note: “NOS” means “Not Otherwise Specified”.

Crude Oil NOS
Tight Oil
Condensate
Bitumen Blend
Bitumen
Refined Product NOS
Fuel Oil NOS
Distillate Fuel Oil

Residual Fuel Oil
Refinery Intermediate
Solvent
Bio-fuel Oil
Bio-Petro Fuel Oil
Natural Plant Oil
Lube Oil
Dielectric Oil
Hydraulic Fluid
Other

Common Vocabulary

While the data model itself is flexible as to what things are called, and what labels, etc can be used, it is very helpful for data sharing if users use the same words when they mean the same thing. This section intends to document some common vocabulary for the various types of data collected. Ideally these names are written exactly the same way in all data sets, though they should be normalized for capitalization. Only ASCII characters should be used for names if possible

Compound Names and Groups

Compound Group Definitions

Compounds can be grouped in various ways -- in this data model, any compound can belong to zero or more groups. Data providers can add any groupings they may find useful. These are a few examples that may be used in the NOAA ADIOS-DB: this is not a complete list.

BTEX

Benzene
Toluene
Ethylbenzene
m&p-Xylene
o-Xylene

n-Alkanes

C8-C44
Pristane
Phytane

PAHs

- Naphthalenes
- Phenanthrenes
- Dibenzothiophenes
- Fluorenes
- Fluoranthene
- Benzonaphthothiophenes
- Chrysenes

PAH-50

Developed for DwH NRDA -- need to get this list from ??

EPA priority PAH

- naphthalene (NAP)
- acenaphthylene (ACY)
- acenaphthene (ACE)
- fluorene (FLU)
- phenanthrene (PHEN)
- anthracene (ANTH)
- fluoranthene (FLTH)
- pyrene (PYR)
- benzo[a]anthracene (B[a]A)
- chrysene (CHRY)
- benzo[b]fluoranthene (B[b]F)
- benzo[k]fluoranthene (B[k]F)
- benzo[a]pyrene (B[a]P)
- benzo[g,h,i]perylene (B[ghi]P)
- indeno[1,2,3-c,d]pyrene (IND)
- dibenz[a,h]anthracene (D[ah]A)

Alkylated single-ring aromatics

- Isopropylbenzene
- Propylbenzene
- 3&4-Ethyltoluene
- 1,3,5-Trimethylbenzene
- 2-Ethyltoluene
- 1,2,4-Trimethylbenzene
- 1,2,3-Trimethylbenzene
- Isobutylbenzene
- 1-Methyl-2-isopropylbenzene

1,2-Dimethyl-4-ethylbenzene
Amylbenzene
n-Hexylbenzene

Alkylated PAHs

Phenanthrenes

Dibenzothiophenes

Alkanes

Biomarkers

Industry Properties

Total Acid Number or Neutralization Number
Reid Vapor Pressure (RVP)
Aniline Point
Cetane Index
Cloud Point
Smoke Point
Need to fill this out...

Bulk Composition

Wax Content
Sulfur Content
Water Content
GC-TPH
GC-TSH
GC-TAH
GC resolved peaks/TPH

Labels

There are any number of labels that can be applied to a given data set. For the purposes of oil spill response, most of these labels will be the various terms used for petroleum products. As some labels only apply to certain product types, it is helpful if we can keep track of what labels might be applied to what product types.

This is a table of labels currently used by NOAA, along with how they are mapped to product types: (Google Spreadsheet)

https://docs.google.com/spreadsheets/d/1dSwTZu46-RcTD8nYCFkPjskYFITOAOh2FQpjjb7Hph8/)

JSON Examples

JavaScript Object Notation (JSON: https://www.json.org/json-en.html) is a text format widely used for sharing structured data between computer systems. While it began with in-browser web applications, it now sees wide use as a storage and interchange format for a variety of applications. NOAA's ADIOS Oil Database uses JSON has an internal data model, storage, and interchange format. Data that conforms to this data model could be stored in any number of other systems (relational database, CSV files, XML), but they all should be convertible to/from this JSON format.

Measurement:

A measurement is a data structure for storing data with an associated unit and unit type, and optionally a range of values and/or standard deviation and replicates.
Back to description

Simple single value:

```
measurement: {value: 3.4,
              unit: "ppm",
              unit_type: "MassFraction"
              }
```

Single value with multiple replicates:

```
measurement: {value: 3.4,
              unit: "ppm",
              unit_type: "MassFraction",
              replicates: 3,
              standard_deviation: 0.1
              }
```

Range of values:

```
measurement: {min_value: 3.4,
              max_value: 3.8
              unit: "ppm",
              unit_type: "MassFraction"
```

```
              }
```

Greater than or equal to a value:

```
measurement: {min_value: 3.4,
              unit: "ppm",
              unit_type: "MassFraction"
              }
```

Record Metadata

Back to Description


```
{
  "oil_id": "EC002234",
  "name": "Access West Winter Blend",
  "Source_id": "HOOPS16F",
  "reference": {"year": 2013,
                "reference":"Hollebone B. 2013. Physical Properties and
                             Behaviour Measurements of Alaskan North Slope
                             [2013] Crude Oil. Environment Canada, Ottawa,
                             Ontario, Canada. May 2013"},
  "sample_date": "2020-03-19",
  "product_type": "crude",
  "location": "Alberta, Canada",
  "location_coordinates": {"type": "Point",
                           "coordinates": [-125.6, 10.1]
                          },
  "api": 20.93,
  "comments": "Via  CanmetENERGY, Natural Resources Canada",
  "labels": [
    "Heavy Crude",
  ],
  ...
}
```


CCME data:

Back to Description


```
{
    "CCME_F1": {
        "value": 15.58,
        "unit": "mg/g",
```

```
        "unit_type": "massfraction"
    },
    "CCME_F2": {
        "value": 50,
        "unit": "mg/g",
        "unit_type": "massfraction"
    },
    "CCME_F3": {
        "value": 193,
        "unit": "mg/g",
        "unit_type": "massfraction"
    },
    "CCME_F4": {
        "value": 40,
        "unit": "mg/g",
        "unit_type": "massfraction"
    },
}
```


ESTS Hydrocarbon Fractions

[Back to Description]


```
"ESTS_hydrocarbon_fractions": {
    "method": "Hollebone, Bruce (2020) Personal communication",
    "GC_TPH": [
        {
            "measurement": {
                "unit": "mg/g",
                "unit_type": "massfraction",
                "value": 15.24
            },
            "name": "n-C8 to n-C10"
        },
        {
            "measurement": {
                "unit": "mg/g",
                "unit_type": "massfraction",
                "value": 14.17
            },
            "name": "n-C10 to n-C12"
        }
    ],
```

```
    "aromatics": [
        {
            "measurement": {
                "unit": "mg/g",
                "unit_type": "massfraction",
                "value": 3.72
            },
            "name": "n-C8 to n-C10"
        },
        {
            "measurement": {
                "unit": "mg/g",
                "unit_type": "massfraction",
                "value": 2.17
            },
            "name": "n-C10 to n-C12"
        },
    ],
    "saturates": [
        {
            "measurement": {
                "unit": "mg/g",
                "unit_type": "massfraction",
                "value": 18.35
            },
            "name": "n-C8 to n-C10"
        },
        {
            "measurement": {
                "unit": "mg/g",
                "unit_type": "massfraction",
                "value": 10.82
            },
            "name": "n-C10 to n-C12"
        },
    ]
}
```


Distillation Data

[Back to description]


```
"distillation_data": {
```

```
    "method": "ASTM D7169",
    "type": "mass fraction",
    "cuts": [
        {
            "fraction": {
                "unit": "%",
                "unit_type": "massfraction",
                "value": 5
            },
            "vapor_temp": {
                "unit": "C",
                "unit_type": "temperature",
                "value": 35
            }
        },
        {
            "fraction": {
                "unit": "%",
                "unit_type": "massfraction",
                "value": 10
            },
            "vapor_temp": {
                "unit": "C",
                "unit_type": "temperature",
                "value": 52
            }
        },
        {
            "fraction": {
                "unit": "%",
                "unit_type": "massfraction",
                "value": 15
            },
            "vapor_temp": {
                "unit": "C",
                "unit_type": "temperature",
                "value": 70
            }
        },
    ],
},
```

SARA Analysis:

Back to description


```
"SARA": {
    "method": "ESTS: 12.11/1.0/M",
    "aromatics": {
        "unit": "%",
        "unit_type": "massfraction",
        "value": 31
    },
    "asphaltenes": {
        "unit": "%",
        "unit_type": "massfraction",
        "value": 16
    },
    "resins": {
        "unit": "%",
        "unit_type": "massfraction",
        "value": 16
    },
    "saturates": {
        "unit": "%",
        "unit_type": "massfraction",
        "value": 37
    }
}
```


Bulk Composition

Back to Description


```
"bulk_composition": [
{
    "measurement": {
        "unit": "%",
        "unit_type": "massfraction",
        "value": 1.6
    },
    "method": "ESTS: 12.11/2.0/M",
    "name": "Wax Content"
},
```

```
{
    "measurement": {
        "replicates": 3,
        "standard_deviation": 0.025166,
        "unit": "%",
        "unit_type": "massfraction",
        "value": 0.9
    },
    "method": "ASTM E203",
    "name": "Water Content"
},
{
    "measurement": {
        "unit": "%",
        "unit_type": "massfraction",
        "value": 4.1
    },
    "method": "ASTM D4294",
    "name": "Sulfur Content"
}]
```


Compounds

[Back to Description]


```
"compounds": [
{
    "groups": [
        "Alkylated Aromatic Hydrocarbons"
    ],
    "measurement": {
        "unit": "ug/g",
        "unit_type": "massfraction",
        "value": 26.184
    },
    "name": "C0-N"
},
{
    "groups": [
        "Alkylated Aromatic Hydrocarbons"
    ],
    "measurement": {
```

```
        "unit": "ug/g",
        "unit_type": "massfraction",
        "value": 94.578
    },
    "name": "C1-N"
},
{
    "groups": [
        "Alkylated Aromatic Hydrocarbons"
    ],
    "measurement": {
        "unit": "ug/g",
        "unit_type": "massfraction",
        "value": 156.59
    },
    "name": "C2-N"
},
{
    "groups": [
        "Alkylated Aromatic Hydrocarbons"
    ],
    "measurement": {
        "unit": "ug/g",
        "unit_type": "massfraction",
        "value": 145.54
    },
    "name": "C3-N"
}]
```


Dispersability

[Back to description]


```
{
    "dispersant": "Corexit 9500",
    "effectiveness": {
        "max_value": 10.0,
        "replicates": 6,
        "unit": "%",
        "unit_type": "massfraction"
    },
    "method": "Swirling Flask Test (ASTM F2059)"
```

```
}
```


Industry Properties

[Back to Description]


```
"industry_properties": [
    {
        "measurement": {
            "unit": "mg/g",
            "unit_type": "massfraction",
            "value": 0.90915
        },
        "name": "Total Acid Number"
    },
    {
        "measurement": {
            "unit": "%",
            "unit_type": "massfraction",
            "value": 3.1904
        },
        "name": "Conradson Carbon Residue"
    },
```