Crude Oil Characteristics Research
Sampling, Analysis and Experiment (SAE) Plan

The U.S. is experiencing a renaissance in oil and gas production. The Energy Information Administration projects that U.S. oil production will reach 9.3 million barrels per day in 2015 — the highest annual average level of oil production since 1972. This domestic energy boom is due primarily to new unconventional production of light sweet crude oil from tight-oil formations like the Bakken in North Dakota, as well as the Eagle Ford and Permian Basins in Texas. This domestically produced energy is important for American energy security and our economic prosperity. In some of these areas, particularly North Dakota, crude oil is moved to market by rail because production has exceeded the capacity of pipelines to move oil from these areas to refineries in the West, Midwest and Northeast. Data from the North Dakota Pipeline Authority indicates daily export volumes by rail from North Dakota have increased over the past few years from 70,000 barrels per day to 700,000.

In seeking to better understand and to mitigate risks associated with frequent and large volume rail transport of crude oil in general and tight oil in particular, the U.S. Department of Energy (DOE) and U.S. Department of Transportation (DOT) commissioned a review of available crude oil chemical and physical property data and literature related to crude oil potential for ignition, combustion, and explosion. A partial list of properties surveyed includes density (expressed as API gravity), vapor pressure, initial boiling point, boiling point distribution, flash point, gas–oil ratio, "light ends" (dissolved gases—including nitrogen, carbon dioxide, hydrogen sulfide, methane, ethane, and propane—and butanes and other volatile liquids) composition, and flash gas composition. Although the review yielded a large database encompassing a wide variety of crude oils and their properties, it also illustrated the difficulty in utilizing available data as the basis for accurately defining and meaningfully comparing crude oils. Reasons for this difficulty include:

- Sample point variability – Samples are collected at various points along the crude oil supply chain that extends from well to refinery gate. A partial list of sampling points (listed in supply chain order) includes well head, separator outlet, "heater-treater" outlet, stock tank, rail or pipeline terminal, and rail tanker (at varying points along the route from terminal to refinery gate). Crude oils—especially lighter varieties—may undergo significant changes in key volatility-related properties as they progress along the supply chain.
- Sampling method variability – Samples are collected using a variety of closed, open, and flow-through methods that vary in effectiveness of capturing 100% of crude oil volatile liquid and dissolved gas constituents. This is especially important in dealing with light crudes, since it means that a given crude sampled at a single supply chain point using a variety of sampling methods could result in a set of samples with significantly different volatility-related properties.
- Analytical method variability – Samples are analyzed using a variety of different methods including those approved by ASTM and other "standard-setting" organizations, modified ASTM methods, and others. Results from different test methods are not necessarily interchangeable.

An important outcome of the review was formal recognition of the wide-ranging variability in crude oil sample type, sampling method, and analytical method, and acknowledgement that this variability limits the adequacy of the available crude oil property data set as the basis for establishing effective and affordable safe transport guidelines. In recognition of the need for improved understanding of transport-critical crude oil and especially tight crude oil properties, this SAE plan was designed to characterize tight and conventional crudes based on key chemical and physical properties, and identify properties that may contribute to increased likelihood and/or severity of combustion events that could arise during handling and transport. In addition to determination of properties via analytical procedures, other proposed Sampling, Analysis and Experiment activities include:

- Use of acquired chemical and physical property data in development of computational models for predicting crude oil behavior in rail transport accident scenarios.
- Execution of experimental activities (including planned fires and full-scale derailment and/or collision events with rail tankers) to validate and/or improve predictive models.

SAE Plan Objectives

Primary plan objectives include:

- Evaluating open versus closed sampling methods, and identifying at least one method that is best suited for acquiring accurately representative samples of crude oils containing significant levels of dissolved gases and/or light (easily volatilized) hydrocarbon liquids.
- Developing a database comprising chemical and physical properties of tight and conventional crude oils—sampled and analyzed under a standard protocol—that enables meaningful oil-to-oil comparison and illustrates how crude oil properties vary:
    - From reservoir to reservoir.
    - Seasonally.
    - Along various supply chain points from well to refinery gate.
    - With time of production from a single well.
- Identifying any consistent and significant chemical and/or physical property differences between tight and conventional crude oils.
- Identifying crude oil chemical and physical properties (including the possible presence of nitrogen and/or other “inerts”) that could contribute to increased likelihood and/or severity of handling/transport-related combustion events.
- Identifying well-site crude oil conditioning system operational parameters that impact transport safety-critical properties, and quantifying the impact of selected parameters by analyzing samples collected upstream and downstream of conditioning systems operating under a range of conditions.
- Assessing sampling and analysis method impacts on vapor pressure, light ends composition, flash point, flash gas composition, and other transport safety-critical properties.
- Using plan outcomes as a basis for evaluating whether chemical and physical properties can or should be included as compliance metrics in a “crude oil safe transport specification.”

SAE Plan Description

The proposed SAE plan comprises a set of tasks intended to encompass a general approach to achieving the above-cited objectives. The plan is not fully comprehensive in that it prescribes types and numbers of crude oil samples needed, but does not call out specific locations at which samples will be collected. Because sample collection logistics will necessarily vary somewhat depending on location-specific requirements, the plan does not include detailed instructions for all aspects of all sample collection activities. The plan is also not intended to be a fully self-contained document, and as such, it incorporates ASTM and other standard procedures by reference. Because tight oil represents the vast majority of crude-by-rail volume, the plan is weighted toward tight oil, but also addresses conventional oil, with the objective of elucidating any significant tight–conventional differences and—if differences are found—assessing their impact on transport risk. The proposed work scope represents a phased approach, in that knowledge gained from completing each task will inform the execution of subsequent tasks, thereby ensuring maximum efficiency in achieving overall plan objectives. Proposed tasks are described below.

Task 1 – Review and Evaluation of New and Emerging Crude Oil Characterization Data
Although the recently completed DOE/DOT-commissioned literature and data review resulted in aggregation of a large volume of publicly available information and data on transport safety-critical tight oil properties, additional data and information are being developed through ongoing studies. Task 1 will identify and evaluate emerging relevant crude oil property and other characterization data, and utilize the data as appropriate to better define and/or improve Tasks 2–6 of the SAE plan.

Task 2 – Sampling Method Evaluation
Five different sampling methods will be evaluated for application to crude oils containing higher concentrations of dissolved gases and volatile liquid hydrocarbons. Samples will be analyzed for volatility and composition, and results will be compared to "baseline" data acquired using the Strategic Petroleum Reserve (SPR) mobile lab. The SPR mobile lab is a small-scale crude oil separator that functions like a commercial-scale well-site separator. The unit is capable of performing vapor pressure measurement, and can also be used to acquire atmospheric pressure-equilibrated vapor and liquid samples that can be separately analyzed. Vapor composition data and other operating parameters are input into an equation-of-state (EOS) model to ascertain a complete compositional analysis of the C_1 through C_{10} fraction, and liquid analysis is used to characterize the C_{10}+ fraction. This method yields an accurate whole oil analysis that includes accurate quantitation of the light ends (including nitrogen, carbon dioxide, and hydrogen sulfide), that often comprise a significant portion of light crude oils. Vapor pressure and light ends composition are the primary evaluation criteria to be used as the basis for measuring sampling method effectiveness.

Results of the sampling method evaluation will inform the choice of sampling method(s) to be used for subsequent tasks, and provide data to support initial equation-of-state modeling efforts. Task 2 samples will be collected at two selected tight oil rail terminals. In addition to tight oil comprising the major portion of rail-transported crude, the rationale for this is that if a specification for safe rail transport of tight crude is developed, compliance with the specification will likely require rail terminal crude sampling and analysis prior to loading. This will necessitate a sampling method compatible with easy, affordable, and reliable execution at a rail terminal, and lessons learned in this initial sample acquisition task will be useful in establishing an appropriate method.

Task 3 – Initial Combustion Experiments and Modeling

Task 3 will be conducted concurrently with Task 2 and comprise combustion experiments and computational modeling to assess combustion hazards associated with tight and conventional crude oils. Key focus will be on 1) identifying crude oil properties that can affect the type and level of hazards associated with a combustion incident, 2) assessing the impact of identified properties, and 3) developing a prioritized list of properties/parameters that need to be included in subsequent crude oil characterization activities. Several crude oil properties are necessary for projecting the risk/hazard level of various combustion events. Table 1 lists combustion events, associated properties, and testing scale required to obtain these properties. In addition to Task 3 testing activities, Table 1 references rail car-scale activities proposed for Task 5. Task 3 tests will be designed to determine these properties for tight and conventional crude oils to enable comparison between the two oil types. The determined properties could then be utilized for thermal hazard calculations for both tight oils and conventional crude oils. These calculations would allow the determination of whether tight oils are different compared to conventional crude oils with regard to combustion hazard severity.

In addition to combustion experiments, computational fluid dynamics (CFD) modeling will be initiated in Task 3 to determine if the dispersion of light volatiles into the atmosphere from tight crude oil is different than from conventional crudes. The evaluation of the vapor cloud extent is important for hazards concerning flash fires and explosions. CFD will be used to simulate the dispersion of light volatiles from tight crude oil and several conventional crude oils. For each oil, vapor cloud extent will be determined, as well as the regions of the lower and upper flammability limits. Simulations will be performed for different environmental conditions and different levels of infrastructure. Data obtained from bench-scale tests measuring gas composition for different levels of heating will be utilized for the simulations.

Table 1 – Combustion Events, Properties Needed for Hazard Analysis, and Scale

Combustion Event	Properties	Scale
Applicable to all events	• Heat of combustion • Flammability limits • Boiling point temperatures of components • Density • Molecular weight • Composition in liquid/gas phases	Small; can be conducted in the laboratory.
Pool fire	• Burn rate • Surface emissive power • Flame height • Heat flux to an engulfed object	1- to 10-meter pool. Bund and free spill.
Fireball/BLEVE*	• Geometry • Surface emissive power • Duration • Fragment characterization (velocities, geometry, range) • Overpressures	Rail car (BLEVE). Rail car or reduced scale (fireball).
Vapor Cloud (flash fire, explosion)	Gas composition	Rail car or reduced scale

* Boiling Liquid Expanding Vapor Explosion

Task 4 – Crude oil Characterization – Tight Oil versus Conventional Oil
In Task 4, previous task outputs and recommendations will be used to generate a concise yet comprehensive data set that accurately characterizes multiple crude oil types. Key focus will be on crude oils at rail or pipeline terminals that are destined for transport to relatively distant refineries. Results from this characterization effort, along with information gathered from combustion testing and modeling, will provide a better understanding of which crude oil properties have the greatest impact on combustion event hazards, and whether and to what extent these properties are preferentially associated with tight rather than conventional oils. Results will also inform the prioritization of subsequent efforts to compare crude oil properties based on geography, seasonal impacts, environmental conditions, well lifetime, and supply chain point.

Task 5 – Large-Scale and Rail Car Combustion Testing and CFD Modeling
Rail tanker tests will be conducted to collect empirical data for validation and/or revision of Task 3-developed computer models for predicting crude oil behavior under combustion and explosion conditions. Validation of predictive model results and/or improving model performance via empirical tests will also help establish which crude oil properties are critical influences on combustion behavior, and inform efforts to prioritize future crude oil characterization activities. In conjunction with experimental activities, CFD analysis will be conducted to provide insight into fireball and Boiling Liquid Expanding Vapor Explosion (BLEVE) behavior.

Task 6 – Comprehensive Sampling, Analysis and Experiment
In addition to better characterization of crude oils at interstate transport rail and pipeline terminals, a better understanding of the factors influencing crude oil properties is needed. Of particular interest are the impacts of varying types and levels of crude oil conditioning on chemical and physical properties of major relevance to combustion behavior. Obtaining the data required to assess these impacts will require access to accurate information regarding how well-site conditioning equipment is operated. Using previous task outputs and recommendations, Task 6 will assemble a comprehensive data set that accurately characterizes crude oils sampled:

- At multiple geographic locations.
- At different points on the production supply chain ranging from well-head to refinery gate.
- In different seasons and at different ambient temperatures experienced throughout the year.
- At different points over the lifetime of a well.

A total of about 160 samples will be collected from five oil plays, at eight points along the production/supply chain, during two separate seasons, and at two different points in the lifetime of a well. The number of samples and extent of analytical activities may be adjusted based on outcomes and recommendations of previous tasks.