Petroleum Substances: Special Considerations for Interpreting HPV Data

Characterizing Chemicals in Commerce:

Using Data on High Production Volume (HPV) Chemicals

December 13, 2006

Thomas M. Gray, M.S., D.A.B.T.

API Technical Manager, Petroleum HPV Testing Group

Petroleum Substance: Special Considerations
Presentation Outline

- **Petroleum HPV Testing Group (TG)**
- **Petroleum Substances**
  - Most Highly Complex Mixtures
  - Major Chemical Classes of Compounds
  - Sources of Compositional Uniqueness, Complexity and Variability
  - Definitions
- **Category Approach for Meeting Data Commitments**
  - Rationale, Grouping, Category Justification, and Methods Used for Predicting Values for Untested Substances
  - TG Categories
- **Impact of Substance Composition on HPV Properties**
  - Physical/Chemical
  - Environmental Fate
  - Ecotoxicity
  - Mammalian Toxicity

Petroleum Substances – Special Considerations
Petroleum HPV Testing Group (TG)

- **60 Member Companies**
  - American Petroleum Institute (Program Administrator)
  - Asphalt Institute
  - Gas Processors Association
  - National Petrochemical & Refiners Association
- **405 Substances**
  - Hundreds of refinery streams in the program because each is isolated at a refinery
  - Multiple product types are blended from the various streams

Petroleum Substances – Special Considerations
Petroleum Substances

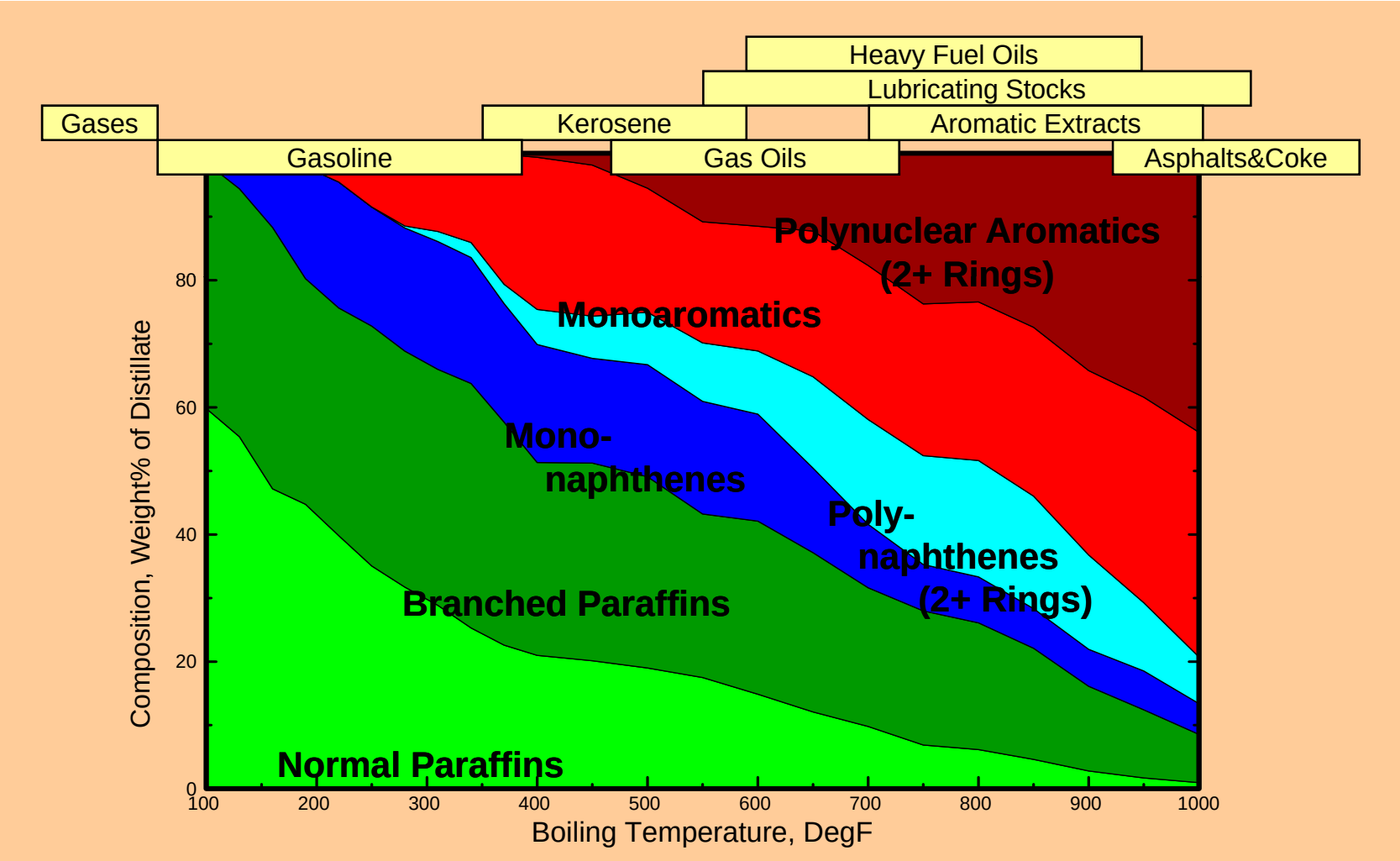
- **Most are complex mixtures (TSCA Class 2 Substances)**
  - "…may have unknown or variable compositions or be composed of a complex combination of different molecules."
  - "…each UVCB can be considered to be category of molecules, often closely related."
- **Compositional variability means most substances will have a range of HPV values**

Petroleum Substances – Special Considerations
Petroleum Substances (cont'd)

- **Major Chemical Classes of Compounds**
  - Saturated linear hydrocarbons (alkanes or paraffins)
  - Unsaturated linear hydrocarbons (alkenes or olefins, etc.)
  - Saturated cyclic hydrocarbons (naphthenes or alicyclics)
  - Unsaturated cyclic hydrocarbons (aromatic hydrocarbons)
  - Heteroatomic compounds (linear and aromatic compounds containing C,H and N, S, O or metals)
  - Inorganic compounds
- **Sources of Compositional Uniqueness, Complexity and Variability**
  - Crude oil source
  - Crude oil distillation temperature
  - Further processing steps

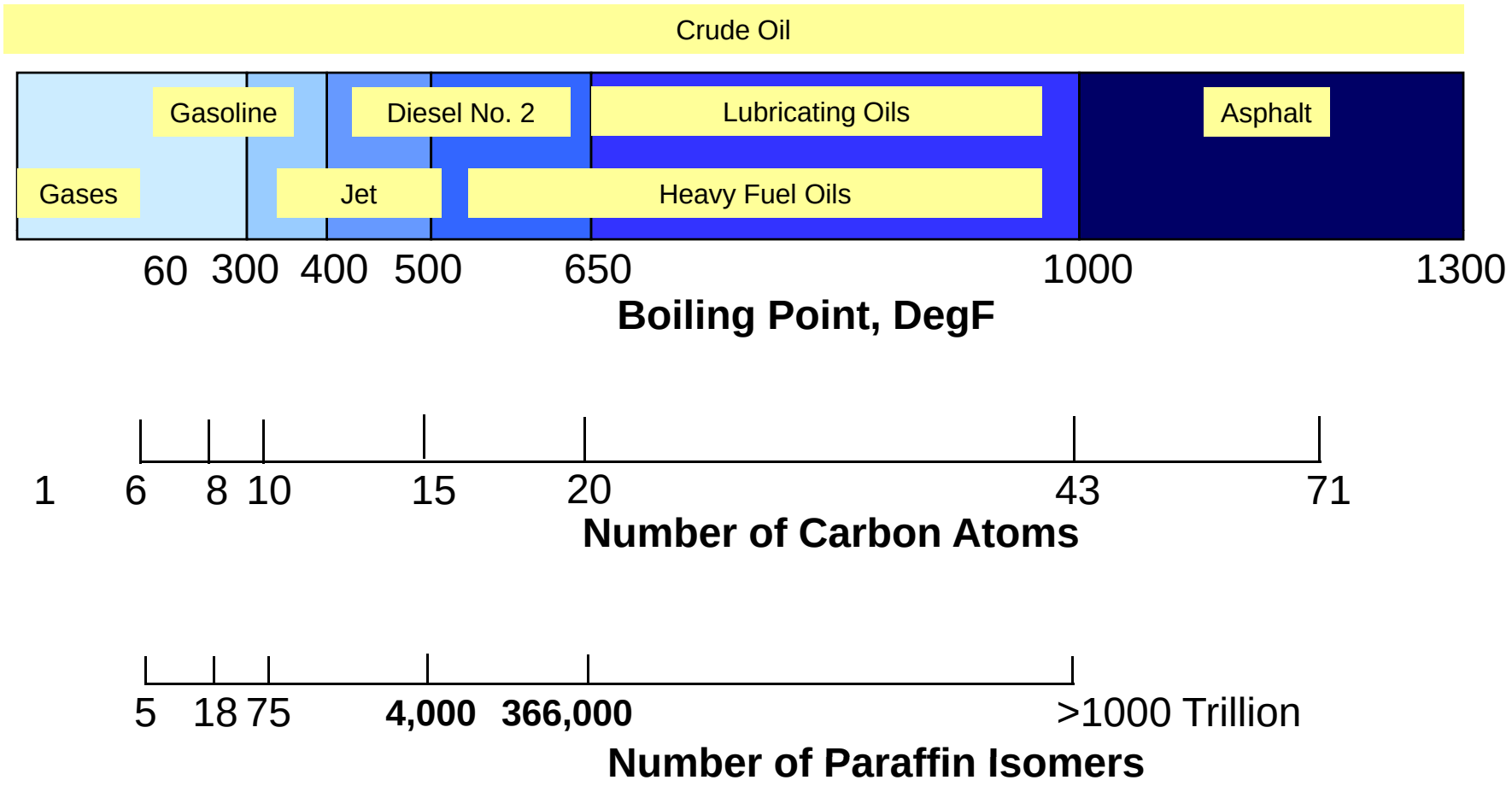
Petroleum Substances – Special Considerations

Petroleum Substances (cont'd)



Petroleum Substances – Special Considerations

Petroleum Substances (cont'd)



Petroleum Substances – Special Considerations

Petroleum Substances (cont'd)

- **Definitions**
  - Hydrocarbon type[1]
  - Last process step[2]
  - Carbon range[3]
  - Boiling range[4]

- **Sample stream name and definition**
  - Distillates (petroleum), hydrotreated light
  - A complex combination of hydrocarbons[1] obtained by treating a petroleum fraction with hydrogen in the presence of a catalyst[2]. It consists of hydrocarbons having carbon numbers predominantly in the range of C9 through C16[3] and boiling in the range of approximately 150°C to 290°C (302°F to 554°F)[4].

Petroleum Substances – Special Considerations
Category Approach for Meeting Data Commitments

- **Rationale for Using Categories**
  - The value of existing data is maximized and new testing is minimized by applying data from tested substances to untested substances
- **Grouping of Category Members**
  - Products and their blending streams
  - Substance definitions are used to group substances
- **Justification of Categories**
  - Category members have similar composition
  - HPV substance properties are function of composition
- **Predictive Methods Used for Applying Existing Data to Untested Substances**
  - Read Across
  - Modeling

Petroleum Substances – Special Considerations
TG Categories

Petroleum Gases
Gasoline
Kerosene/Jet Fuel
Gas Oils
Heavy Fuel Oils
Lubricating Oil Basestocks
Aromatic Extracts
Petroleum Waxes
Asphalt
Petroleum Coke
Crude Oil

Lubricating Grease Thickeners
Reclaimed Substances
- Hydrocarbons
- Naphthenic Acids
- Disulfides
- Acids/Caustics

Petroleum Substances – Special Considerations

Impact of Substance Composition on Physical/Chemical Properties

Example - Log K_{ow} Value For Kerosene/Jet Fuel

Class	C9	C16
n-paraffin	4.8	**8.2**
iso-paraffin	4.7	8.1
mono-olefin	5.2	8.1
1-ring cycloparaffin	4.6	8.0
2-ring cycloparaffin	3.7	7.1
1-ring aromatic	3.7	7.4
2-ring aromatic	**3.3**	6.2

Petroleum Substances – Special Considerations
Impact of Substance Composition on Environmental Fate Properties

Example - Hydrolysis of an organic chemical is the transformation process in which a water molecule or hydroxide ion reacts to form a new carbon-oxygen bond.

Technical Discussion Rather Than Discrete Data

The chemical components that comprise the kerosene/jet fuel category are hydrocarbons that are Not Subject To Hydrolysis because they lack functional groups that hydrolyze.

Petroleum Substances – Special Considerations
Impact of Substance Composition on Toxicity Testing

- **Ecotoxicity**
  - Experiments conducted and reported as water accommodated fractions or loading rates
- **Mammalian**
  - Route of administration appropriate for human risk assessment
    - Inhalation
    - Dermal

Petroleum Substances – Special Considerations
For more information

- http://www.epa.gov/HPV/
- Tom Gray: grayt@api.org