PKI MN Method: Assessing and Validating a New Method of Knocking Characteristic Determination for LNG as Fuel

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Gas quality (1)

- Gaseous fuels are gaining more interest to be used in engines for transportation and power generation
- Motivating factors compared to liquid fuels (e.g. Diesel, HFO etc.):
  - Environmental benefits (soot, NO$_x$, CO$_2$, sulfur etc.)
  - More stringent legislation (e.g. ECA zones ships)
  - Fuel costs
  - World wide availability

Source: BP Energy Outlook 2017
Gas quality (2): what sources are available and what are the future trends?

- Traditional gaseous fuels used in engines
  - Natural gas
  - Biogas
  - Liquid natural gas (LNG);

- Trend towards gaseous fuels to be used in engines
  - Liquid petroleum gas (LPG) as shipping fuels
  - Ethane as shipping fuel
  - Hydrogen blending (pipeline gas)
  - Wellhead gases (contains C₅+);

- All these different sources have substantial different gas compositions
Due to differences in (natural) gas sources, production technologies and the target markets the composition may vary substantially.

Alaska gas: 100% CH₄

Shale gas (US): 84% CH₄, 16% C₂H₆

Peruvian gas: 89% CH₄, 10.5% C₂H₆, 0.5% N₂

Dutch gas:
- 83.5% CH₄
- 2% C₂H₆
- 0.5% C₃H₈
- 1% C₄H₁₀

Russian gas 1 (e.g.):
- 92% CH₄
- 5% C₂H₆
- 2% C₃H₈
- 1% C₄H₁₀

Russian gas 2 (e.g.):
- 100% CH₄

Qatar gas:
- 91% CH₄
- 6.5% C₂H₆
- 1.5% C₃H₈
- 0.7% C₄H₁₀
- 0.33% N₂

Australian gas:
- 88% CH₄
- 10% C₂H₆
- 2% C₃H₈

Source: Includes data from CEDIGAZ, CISStat, GAIL, IHS CERA, Poten, Waterborne.
Gas composition variations in practice

Methane number e.g. 65-100
variation of 35 points

Octane number 95 or 98 (Neth.)
Isooctane as industry standard
Narrow bandwidth
Gas composition variations, so what?

- Different LNG compositions have different **combustion properties**: most critical for engine performance is resistance to engine knock.

- Engine knock is caused by **unwanted** autoignition of unburned fuel-air mixture (end gas).

- The occurrence of **engine knocking** leads to significant loss of performance (power reduction), increase in CO$_2$ emissions, potential engine shutdown and potentially extensive damage!
**Engine knock: methane number**

- Knock “resistance” is critical fuel (gas) property expressed in **methane number** (MN)
- 0-100 scale analogous to the octane number for gasoline.
- Engines are designed/tuned for fuel with given **methane number** to **maximize engine performance**
- Too low **methane number** induces engine knock causing significant loss of performance (power reduction), potential engine shutdown and potentially extensive damage!
- Different engine designs and/or adjustments translate into different sensitivities to knock with variations in fuel composition
- “Wrong” fuel in “wrong” engine = trip/damage and bad rep
## Overview methane number tools

<table>
<thead>
<tr>
<th>Name</th>
<th>Based on</th>
<th>Gas range</th>
<th>Available as</th>
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</table>
| AVL  | Experimental data using stoichiometric test engine | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/N<sub>2</sub>/H<sub>2</sub>/CO/CO<sub>2</sub>/H<sub>2</sub>S/O<sub>2</sub> (C<sub>2</sub>/C<sub>6</sub>=C<sub>4</sub>; no isomer discrimination) | 1. Calculation tool (fee)  
2. Test data |
| MWM (published in the standard EN 16726, 2015) | AVL data + MWM experimental data | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/C<sub>5</sub>/C<sub>6</sub>/N<sub>2</sub>/H<sub>2</sub>/CO/CO<sub>2</sub>/H<sub>2</sub>S/O<sub>2</sub>/H<sub>2</sub>O (no isomer discrimination) | 1. Online calculation tool (no fee)  
2. (Complex) algorithm in annex of EN 16726 |
| DGC  | AVL data | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/N<sub>2</sub>/H<sub>2</sub>/CO/CO<sub>2</sub> (C<sub>2</sub>/C<sub>6</sub>=C<sub>4</sub>; no isomer discrimination) | Online calculation tool (fee) |
| DNV GL & SHELL LNG PKI-MN | Combustion/auto-ignition model w. experimental verification | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/C<sub>5</sub>/N<sub>2</sub> (w/ isomer discrimination) | 1. Online calculation tool (no fee)  
2. (Simple) algorithm |
| DNV GL Pipeline PKI-MN | Combustion/auto-ignition model w. experimental verification | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/C<sub>5</sub>/C<sub>6</sub>/N<sub>2</sub>/CO/CO<sub>2</sub>/H<sub>2</sub>/H<sub>2</sub>S (w/ isomer discrimination) | 1. Online calculation tool (no fee)  
2. (Simple) algorithm |
| Cummins-Westport | ?? | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/C<sub>5</sub>/mix-C<sub>6</sub>/mix-C<sub>7</sub>/n-C<sub>8</sub>/N<sub>2</sub>/H<sub>2</sub>/CO/CO<sub>2</sub>/H<sub>2</sub>S/O<sub>2</sub> | Online calculation tool (no fee) |
| Wärtsilä (PKI MN) | Combustion/auto-ignition model w. experimental verification | C<sub>1</sub>/C<sub>2</sub>/C<sub>3</sub>/C<sub>4</sub>/C<sub>5</sub>/mix-C<sub>6</sub>/mix-C<sub>7</sub>/n-C<sub>8</sub>/N<sub>2</sub>/H<sub>2</sub>/CO/CO<sub>2</sub>/H<sub>2</sub>S (w/ isomer discrimination) | Online calculation tool (no fee) |

And many more....
Several methane number calculation methods are available

- Methane number: e.g. 65-100
- Octane number 95 or 98 (Neth.)
- Isooctane as industry standard
- Cetane number min. 41 (road transport)

Unlike other transportation fuels, there are currently no standards relating to the properties of LNG to guarantee its safe and efficient use.

These methane number methods give different outcomes for the same fuel composition, which results in confusion for end users and fuel suppliers in the LNG value chain.

- ISO group “Specifications of LNG as marine fuel”:

  End of this year: ISO standard on methane number (PKI MN and MWM)
Why did DNV GL develop their own methane number tool? Are existing methods not fit for purpose?

**AVL methane number tool**
- Based on data published by AVL in 1971
- Data generated for a stoichiometric engine
- Higher hydrocarbons up to only butane
- Data and fitting based on triangular diagrams
- “Black box”
- **Complex** algorithm (based fitting, relatively slow process)
- Most other methods (e.g. MWM) are based on the experimental AVL dataset

**Market trend new gases**
- Trend towards high BMEP and **ultra lean burn engines**
- Use of wellhead gases in gas engines: contains **substantial fractions of C₅⁺**
- **Greening of pipeline gas**: introduction biogas (**CH₄/CO₂**) and hydrogen
- **Dedicated, fast and easy to use** knock algorithm for integration in fuel adaptive engine control systems

Mismatch between AVL and future gases/engines!
Development of the gas only input knock algorithm
What is knock and how to predict engine knock?

Knock is autoignition of end gas

- competition between propagating flame front and autoignition reactions in end gas
- impacted by changes in fuel composition
- autoignition chemistry, burn rate and heat capacity
**Modelling approach DNV GL**

1. **Engine details (CR, bore, λ, etc.) and gas composition**

2. **Phasing model**

3. **Ignition model**

4. **Knock characterization**

5. **Thermodynamics**
   - Chemical kinetics

6. **Engine knock model is tested and optimized based on experiments using the MAN engine in the DNV GL test lab**
**Experimental setup and test program**

- **Make** - MAN - E2876LE302
- **Rated power** - 208 kW
- **Rated speed** - 1500 rpm
- **Bore x stroke** - 128 x 166 mm
- **C.R.** - 11 : 1
- **Configuration** - 6 cyl. in-line, turbocharged-intercooled
- **Combustion** - spark ignition, open chamber, lean-burn

### Gas composition analysis
- Ethane ($\text{C}_2\text{H}_6$)
- Propane ($\text{C}_3\text{H}_8$)
- Butane (i & n-$\text{C}_4\text{H}_{10}$)
- Nitrogen ($\text{N}_2$)

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**Mixing station**

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PKI methane number accurately predicts knock behaviour... whereas other methods show significant spread.
Comparison with other methane numbers methods

Traditional methods

- Based on experimental work done on stoichiometric engine from 1970s
- **Complex relations** to determine methane number (fitting with dedicated solver)
- Effect of some species ($N_2$, isomers of butane and pentane) neglected

PKI MN methane number

- Based on experimental work done on modern lean-burn engine
- **Straight forward** polynomial equation (fast!):

\[ PKI = \sum \alpha_i n X_i^n + \sum \beta_i n_{*j} m X_i^n X_j^m \]

(X = mole fraction, $\alpha, \beta =$ coefficients)

- Effect of all species relevant for LNG included ($N_2$, isomers of butane and pentane)
**Online algorithm:**

http://pkicalculator.dnvgl.com/pipeline-gas/

**Background information and LNG algorithm:**

Benefits of combining algorithm with (fast) gas quality sensors
Development of smart combustion control systems to improve efficiency and the use of a wide range of fuels

▪ Sensors/Analyzers:
  – Real-time gas composition measurement
  – Fit for purpose, response time, accuracy

▪ Novel Algorithms:
  – Combustion control algorithms based on fuel gas composition and operational conditions of installation
  – Taken into account external factors (e.g. humidity, temperature, etc)

▪ Optimal equipment performance:
  – Fuel adaptive control for a wide range of fuel compositions
  – Safe and reliable operation within a wide range of gas compositions
  – Fuel savings
  – Acceptable emission levels
Fuel-adaptive engine control

Together with Shell, DNV GL developed an engine control system for feed-forward optimization engine performance:

- Fuel composition sensor
- Combustion algorithms (engine knock)

Engines are design and adjusted to operate on the least knock resistant fuel at the expense of lower power and efficiency, and increased emissions.
Fuel-adaptive engine control

Benefits:

- Engine can handle a broad range of gas composition
- Up to 5% fuel consumption saving

Source: MKS Instruments website
Summary

- DNV GL and Shell developed an easy to implement verified open source algorithm for LNG gases: **PKI Methane Number**
- The PKI Methane number tool **outperforms** existing tools like AVL- and MWM MN regarding accuracy, number- and range of fuel compositions that can be calculated.
- In contrast to existing algorithms the PKI Methane Number algorithm can be easily integrated into fast response gas sensors. This allows real time fuel adaptive engine control and determination of the methane number during bunkering.

- Fuel-adaptive engine control system can achieve substantial fuel savings (**5% in tests at DNV GL lab**)
- The algorithm can be easily expanded to other fuels (and incorporation of weather conditions) and engine platforms by performing only a limited number of measurements.
Testing and optimizing chemical mechanism to predict autoignition behavior of fuels at engine conditions

- Optimization chemical mechanism at engine conditions is performed based on >>1000 measurements in a Rapid Compression Machine (pressures up to 100 bar)

<table>
<thead>
<tr>
<th>Pure fuels</th>
<th>(\text{CH}_4, \text{C}_2\text{H}_6, \text{n-}\text{C}<em>4\text{H}</em>{10}, \text{i-}\text{C}<em>4\text{H}</em>{10} \text{ and } \text{H}_2)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Binary mixtures</td>
<td>(\ldots\text{C}_2\text{H}_6, \text{C}_3\text{H}_8, \text{n-}\text{C}<em>4\text{H}</em>{10}, \text{i-}\text{C}<em>4\text{H}</em>{10}, \text{n-} \text{C}<em>6\text{H}</em>{12}, \text{i-}\text{C}<em>6\text{H}</em>{12}, \text{neo-}\text{C}<em>5\text{H}</em>{12}, \text{H}_2, \text{CO}, \text{N}_2\text{ and } \text{CO}_2, \text{H}_2\text{S})</td>
</tr>
<tr>
<td>Ternary mixtures</td>
<td>(\ldots\text{H}_2\text{ and CO})</td>
</tr>
<tr>
<td>Pipeline fuels</td>
<td>Dutch natural gas</td>
</tr>
</tbody>
</table>
Examples of RCM measurements and simulations

- Disagreement at high pressures larger than 40%
- After optimization agreement better than 15%