Flash points of gasoline from Kukersite oil shale: Prediction from vapor pressure

R. Rannaveski and M. Listak[*]

Tallinn University of Technology, School of Engineering, Department of Energy Technology, Ehitajate tee 5, EE19086 Tallinn, Estonia
[*]Correspondence: madis.listak@ttu.ee

Abstract. The flash point of liquid fuels, especially of light distillates such as gasoline or naphtha, is an important parameter for the handling of such materials. In this work, flash points and volatility characteristics (vapor pressure, boiling point) of a number of shale gasoline samples with different volatilities were measured. The shale gasoline fractions were produced from Kukersite oil shale using solid heat carrier retorting technology. Several existing correlations for calculating flash points of hydrocarbons and petroleum fractions are evaluated, and the absolute average deviations were found to be between 1.1 to 20.9 °C. New, easy-to-use correlations are proposed for estimating flash points for oil shale based gasolines from volatility characteristic that are readily available. The correlation proposed in this work are based on the vapor pressure at 20 or 37.8 °C (100 °F), Reid vapor pressure (37.8 °C) or boiling point. The average absolute deviations for these correlations were 0.82 to 0.93 °C, meaning they are comparable to or better than existing methods developed for petroleum oils, which mostly use boiling point as the input parameter, when applied to gasoline from Kukersite oil shale.

Key words: oil shale, gasoline, flash point, closed cup, correlations, vapor pressure, Reid vapor pressure, boiling point, alternative fuel, mineral oil.

INTRODUCTION

Oil shale (a solid fossil fuel) has the potential to be an important source of liquid fuel due to the large amount of oil shale resources available worldwide (Oja & Suuberg, 2012). The world's oil shale resources are estimated to be equivalent to more than 2.9 trillion barrels of oil (1 barrel = 0.159 m^3) (Dyni, 2003). Shale oil is obtained by thermally processing kerogen, the insoluble crosslinked organic matter in oil shale (Savest et al., 2007; Hruljova et al., 2013). This is performed in an oxygen free environment in a process termed pyrolysis (also known by the industrial term 'retorting'). The process results in a so called 'synthetic crude oil', which, similarly to tars/oils from coal or biomass pyrolytic thermochemical conversions (Suuberg & Oja, 1997; Oja & Suuberg, 1998), has a wide distribution of properties/constituents (for kukersite oil shale derived shale oils see Oja, 2005; Oja, 2015; Oja, 2015a; Järvik & Oja, 2017). Therefore, in industry commonly the 'synthetic crude oil' is divided into 'straight-run fractions' as products (Qian, 2010). Often one of these products is a shale gasoline fraction with a boiling range up to about 200 °C (Oja, 2007; Qian, 2010). As with

petroleum based gasoline, the handling of shale gasoline depends on several parameters, one of which is the flash point. Knowledge of a flammable liquid's flash point is an important factor in the production, processing, handling and transport of these liquids because it describes the fire and explosion potential of a material (Hristova & Tchaoushev, 2006; Skrinska et al., 2015). Fuels with low flash points have a higher fire hazard. The flash point is also a key parameter for the classification of flammable liquids, and is an important parameter included on material safety data sheets (MSDS). The flash point is defined as the lowest temperature at which there is enough vapor to ignite a mixture of air and these vapors. Therefore, in addition to technical constraints (experimental methods/procedures (Phoon et al., 2014)), the flash point value depends in large measure on vapor pressure of a substance, but also somewhat on its composition/structure. There are various prediction methods available for flash points, varying from simple empirical methods with one input parameter to more sophisticated methods (Hristova & Tchaoushev, 2006; Valenzuela et al., 2011; Phoon et al., 2014). However, for oils and oil fractions (ill-defined mixtures that can contain from hundreds to thousands of components) mostly one input parameter based empirical methods are of practical interest (see Table 1).

In this paper the practical interest is in evaluating the close cup flash points of the 'straight run' gasoline fraction (ill-defined mixture) from Kukersite shale oil. For this particular shale oil, produced by solid heat carrier (SHC) retorting technology from Kukersite oil shale, about 20% of the shale oil is taken as the gasoline fraction, which has a boiling range below 200 °C. The shale gasoline consists mainly of paraffins and olefins (67%). It also contains compounds containing heteromatoms, such as sulphur or oxygen, as the content of heteroatoms is about 2–4% (Gubergrits et al., 1989; Qian, 2010). Some background information on thermodynamic properties of shale oil gasolines can be found from (Kollerov, 1951; Qian, 2010; Baird & Oja, 2016). The aim of this work was to provide convenient predictive correlations for determining the flash point of this shale gasoline from its vapor pressure at a certain temperature (vapor pressure at 20 °C or Reid vapor pressure at 100 °F) or its atmospheric boiling point. In addition to proposing new correlations, we also test the applicability of existing flash point correlations that have been proposed for hydrocarbons or petroleum fractions. The correlations tested are given in Table 1. A more detailed description of some of these correlations, and several other correlations that use different input parameters than what we tested in this work, can be found in (Alqaheem et al., 2017).

EXPERIMENTAL

Materials
The shale gasoline fractions used in this study were obtained from the whole shale oil (Kollerov, 1951; Baird et al., 2015; Oja et al., 2016) produced using a solid heat carrier process (Golubev, 2003; Elenurm et al., 2008) at Eesti Energia's Narva Oil Plant (Narva, Estonia). This plant uses Kukersite oil shale (Estonia) as the raw material. Two different gasoline fractions were used, which were produced at different times. The gasoline fractions are henceforth identified as Sample 1 (specific gravity (SG) of 0.751, atomic hydrogen-carbon ratio (H/C) of 1.82) and Sample 2 (SG 0.77, H/C 1.81). From these, different shale gasoline samples with varying volatility were prepared by evaporating part of the sample in a simple batch distillation system (similar to the setup

for an Engler distillation (ASTM D86). In total 8 samples were prepared for further analysis, with 7 to 38% of the gasoline being evaporated. These samples were used for vapor pressure and flash point measurements. The flash points of the initial shale gasoline fractions (Sample 1 and Sample 2) were ≤ -38 °C.

Closed cup flash point measurements

The flash points were measured according to the ASTM D6450 closed cup flash point standard. Measurements were carried out using an Eralytics Eraflash Flash Point Tester. It was found that due to the limitations of our Eraflash flash point tester measurements for samples with flash points below -10 °C were less accurate than measurements for the other samples. The standard deviation for samples with flash points greater than -10 °C was below 1 °C. However, for samples with flash points lower than -10 °C, the standard deviation was found to be up to 2.1 °C. Therefore, more measurements had to be carried out to get a more accurate average flash point and the flash points reported in this study are average values of five measurements. The performance of the setup was tested using dodecane and benzene (Sigma-Aldrich, purity > 99%). Using the Eraflash Flash Point Tester the flash point of dodecane was found to be 78.5 ± 0.5 °C, which is comparable to the flash point found in the literature (81–83 °C (Hughes et al., 1996; Li et al., 2014)); the flash point benzene was found to be -0.8 ± 0.5 °C, which is comparable to the flash point found in literature (-13 to -9 °C (Mack, 1923; Choe, 1988)); the flash point of toluene was found to be 8.2 ± 0.5 °C, which is comparable to the flash point found in literature (7.2 °C (Liaw et al., 2010)).

Vapor pressure measurements

The vapor pressure curves covering the temperature range from room temperature to 100 °C were measured using a commercial Eralytics Eravap Vapor Pressure Tester according to the ASTM D6378 Standard. Performance tests for the device can be found in (Siitsman & Oja, 2015). Some earlier vapor pressure data also exist for Kukersite shale gasoline fractions with narrow boiling ranges (Siitsman & Oja, 2015), which were measured using the DSC technique (Siitsman et al., 2014; Siitsman & Oja, 2016).

RESULTS AND DISCUSSION

Because the aim of this work was to derive/propose easy-to-use correlations for the determination of the flash point from a convenient volatility characteristic (such as the vapor pressure at a specific temperature or the boiling point), the vapor pressures of the shale gasoline samples were measured. For the 8 samples the exact evaporation percentages and vapor pressure data are given in (Table 2).

Table 1. Overview of existing flash point (TF) correlations, containing either boiling point (TB) or vapor pressure (pvap) as input parameters, tested in this work

Corre-lation	Authors	Equation	Range	Ref
1	Butler et al.	$T_F(°K) = 255.752 T_B(°K) - 119$	$366.2 \leq T_B \leq 644.2°K$	(Butler et al., 1956)
2	Riazi-Daubert	$\dfrac{1}{T_F 0.556(°K)} = -1.4568 * 10^{-2} + \dfrac{2.84947}{0.556 T_{B(°K)}} - 1.057 * 10^{-3} ln T_B(°K)$	$338.2 \leq T_B \leq 866.2 °K$	(Riazi & Daubert, 1987)
3	Walsh-Mortimer	$T_F(K) = 231.2 - 40 \log(p^{vap}(310.93 °K)) \, (bar)$	N/A	(Walsh & Mortimer, 1971)
4	Patil	$T_F(K) = 4.656 + 0.844 T_B - 2.34 * 10^{-3} T_B^2$	$248.15 \leq T_F \leq 381.48°K$	(Patil, 1988)
5	Satyanarayana-Kakati	$T_F(°K) = -83.3362 + 273.73 T_B(°K) + 0.1118 * \dfrac{10^{-3}}{274.15 T_B(°C)} + 38.734 SG$	$293.2 \leq T_B \leq 613.2 \ K$	(Satyanarayana & Kakati, 1991)
6	Satyanarayana-Rao (hydrocarbons)	$T_F(K) = 225.1 + \dfrac{537.6 \left(\dfrac{2217}{T_B(K)}\right)^2 e^{-\frac{2217}{T_B}}}{\left(1 - e^{-\frac{2217}{T_B}}\right)^2}$	N/A	(Satyanarayana & Rao, 1992)
7	Satyanarayana-Rao (petroleum fractions)	$T_F(K) = 237.9 + \dfrac{334.4 \left(\dfrac{1807}{T_B(K)}\right)^2 e^{-\frac{1807}{T_B}}}{\left(1 - e^{-\frac{1807}{T_B}}\right)^2}$	N/A	(Satyanarayana & Rao, 1992)
8	Hshieh (Organic)	$T_F(°K) = -54.5377 + 273.7383 T_B(°K) + 0.00022 T_B^2$	$263.2 \leq T_B \leq 648.2 \ K$	(Hshieh, 1997)
9	Hshieh (Organosilicon)	$T_F(°K) = -51.2385 + 273.6494 T_B(°K) + 0.00047 T_B^2$	$263.2 \leq T_B \leq 648.2 \ K$	(Hshieh, 1997)
10	Alqaheem-Riazi (Hydrocarbons)	$T_F(K) = 0.71 T_B(K)$	$393.0 \leq T_B \leq 707.0 \ K$	(Alqaheem & Riazi, 2017)
11	Alqaheem-Riazi (Petroleum Fractions)	$T_F(K) = 0.69 T_B(K)$	$393.0 \leq T_B \leq 707.0 \ K$	(Alqaheem & Riazi, 2017)
12	Wang-Sun	$T_F(K) = 33.176 + 0.67465 T_B(K)$	N/A	(Wang & Sun, 2001)

SG stands for the specific gravity.

Table 2. Vapor pressure data for initial Sample 1, initial Sample 2 and the samples obtained from evaporating different percentages of these initial shale gasoline samples

T, °C	Sample 1 VP, kPa	Vaporized from Sample 1 7.1% VP, kPa	12.0% VP, kPa	16.6% VP, kPa	24.8% VP, kPa	37.8% VP, kPa	Sample 2 VP, kPa	Vaporized from Sample 2 13.6% VP, kPa	19.2% VP, kPa	23.6% VP, kPa
20	18.9	10.9	8.2	–	–	–	18.1	–	–	–
30	25.9	15.4	12.1	11.0	9.5	–	25.2	9.8	7.2	6.5
37.8	32.9	20.1	16.0	14.7	12.8	9.2	32.2	13.1	9.8	8.9
40	35.2	21.7	17.3	15.9	13.9	10.3	34.5	14.3	10.8	9.7
50	46.7	29.9	24.4	22.5	19.7	15.3	46.1	20.2	15.4	13.9
60	61.2	40.6	33.6	31.3	27.5	21.7	60.5	28.0	21.7	19.6
70	78.9	54.3	45.7	42.6	37.6	30.3	70.8	38.2	30.0	27.1
80	100.5	71.5	61.0	57.2	50.7	41.5	99.0	51.1	40.7	36.9
90	126.8	93.1	80.5	75.8	67.5	56.2	124.3	67.5	54.4	49.5
100	158.5	119.8	104.7	99.0	88.8	74.8	154.6	87.8	71.8	65.7

The calculated volatility characteristics (vapor pressures at 20 and 37.8 °C (100 °F), Reid vapor pressure at 100 °F and the atmospheric boiling point) and measured flash points for the samples are given in (Table 3). These four volatility characteristics were chosen because they are the most common volatility parameters given in gasoline safety data sheets. Vapor pressures at each temperature and atmospheric boiling points were calculated using the data given in (Table 2). For this the dataset corresponding for different evaporation percentages were fitted by an integrated Calusius-Clapeyron equation. Reid Vapor Pressure was calculated from the vapor pressure at 37.8 °C using the following equation (1) from ´ASTM D6377´:

$$RVP = 0.915VP37.8\ °C \qquad\qquad (1)$$

where RVP is the Reid vapor pressure and VP37.8 °C is the measured vapor pressure at 37.8 °C.

The measured flash points were used along with the selected volatility characteristics in Table 3 to develop correlations. Here it is also worth mentioning that when extrapolating to calculate the vapor pressure at the flash point temperature it was found that for shale gasoline the vapor pressure at the flash point was between 1.5 to 2.5 kPa. This is in the range of lower and upper flammability limits (0.01 < Pvap (atm) < 0.08) proposed by ´Algunaibet et al., 2016´.

Table 3. Flash points (T_F) and selected vaporization characteristics of the different samples, obtained from evaporating different percentages of these initial shale gasoline samples. The vaporization characteristics are vapor pressure at 20 °C ($VP_{20\ °C}$), vapor pressure at 37.8 °C or 100 °F $_{(VP100\ °F)}$, Reid vapor pressure (RVP) and boiling point (T_B)

	Based on the initial Sample 1					Based on the initial Sample 2		
Evaporated, %	7.1	12.0	16.6	24.8	37.8	13.6	19.2	23.6
T_F, °C	-14.0	-10.3	-7.7	-4.7	0.5	-6.7	0.5	2.2
$VP_{20\ °C}$, kPa	10.7	8.1	7.3	6.3	4.4	6.5	4.8	4.3
$VP_{100\ °F}$, kPa	20.2	16.1	14.7	12.8	9.4	13.1	9.8	8.9
RVP, kPa	18.5	14.7	13.4	11.7	8.6	12.0	9.0	8.1
T_B, °C	93.5	98.9	101.3	105.8	111.1	105.5	113.5	117.5

The aim of developing correlations using these different input parameters was to make it possible to estimate flash points for shale gasoline from a wider range of available data (either from vapor pressure at 20 or 37.8 °C, the Reid vapor pressure at 100 °F or the atmospheric boiling point). As an illustrative example, Fig. 1 illustrates the relation between flash point and vapor pressure at 20 °C for the shale gasoline fractions studied in this work. As seen from Fig. 1, the flash point-vapor pressure dependency for shale gasoline fractions derived from vaporizing portions of either Sample 1 or Sample 2 show a similar trend.

As seen from Fig. 1, a linear equation can be used to describe the relationship between the flash point and the vapor pressure at 20 °C. This is also the case for other pairs. The following are the linear Eqs (2, 3, 4) correlating the flash point with vapor pressures at 20 and 37.8 °C and the Reid vapor pressure:

$$T_F\ (°C) = -2.6547 VP_{20\ °C}(kPa) + 12.14 \qquad\qquad (2)$$

$$T_F\ (°C) = -1.4948 VP_{100\ °F}(kPa) + 14.337 \qquad\qquad (3)$$

$$T_F \, (°C) = -1.6337 RVP(kPa) + 14.337 \qquad (4)$$

The correlation between the flash point and the boiling points of shale gasoline turned out to be similar to the one proposed by 'Alqaheem and Riazi, 2017' in Eq. 5:
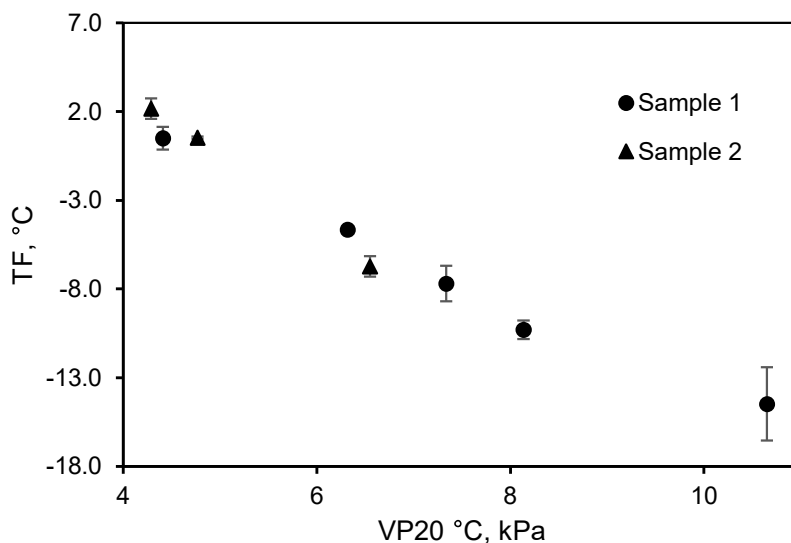
$$T_F(K) = 0.7068 T_B(K) \qquad (5)$$

Figure 1. Graphical representation of the relationship between the flash point (T_F) and the vapor pressure at 20 °C ($VP_{20\,°C}$). Error bars represent the standard deviation of the experiments.

Table 4 summarizes an evaluation of the performance of flash point correlations given in Table 1 when applied to the shale gasoline fractions of this study, and also includes the correlations proposed in this work. The evaluation is based on the average deviation (AD) and absolute average deviation (ADD) of the values predicted by the correlations:

Table 4. Average deviation (AD) and absolute average deviation (ADD) of the calculated flash points, using the correlations from Table 1, when compared to experimental values of this work

	Correlations from Table 1											
	1	2	3	4	5	6	7	8	9	10	11	12
AD, °C	-5.8	-6.2	0.8	6.4	-13.7	-10.6	-22.4	-15.5	-12.2	-1.2	6.4	-21.0
AAD, °C	5.8	6.1	1.1	10.2	13.7	10.6	21.7	15.5	12.2	1.3	6.4	20.9

Deviation = Experimental − Calculated.

Results presented in Table 4 and Table 5 show that Correlations 3 and 10 (from Table 1) and the ones proposed in this work are the most accurate when estimating the flash points of shale gasoline. All these correlations have AADs around 1 °C. On the other hand, Correlations 7 and 12 gave AADs of over 20 °C. Correlations developed specifically for petroleum fractions were also less accurate than their counterparts that were developed for pure hydrocarbons (Correlations 6 vs 7 and 10 vs 11).

Table 5. Average deviation (AD) and absolute average deviation (ADD) of the calculated flash points, using the correlation derived in this study, when compared to experimental values of this work

	Correlations in this work			
	T_B	$VP_{20\,°C}$	$VP_{100°F}$	RVP
AD, °C	0	0	0	-0.2
AAD, °C	0.87	0.93	0.82	0.90

Deviation = Experimental – Calculated.

CONCLUSION

The aim of this work was to propose correlations for estimating the close cup flash point for shale gasoline fraction produced from Kukersite oil shale. These correlations can be used in risk assessment calculations related to handling and transporting these fuels. The work was based on experimentally measured closed cup flash points and vapor pressure curves. Based on the vapor pressure data the desired volatility properties (vapor pressures at 20 and 37.8 °C (100 °F), Reid vapor pressure at 100 °F and the atmospheric boiling point) were determined for 8 gasoline samples with different volatilities. Using this data, convenient correlations were developed or selected from the literature that allow the flash point of Kukersite shale gasoline to be estimated with an AADs of around 1 °C.

REFERENCES

Algunaibet, I.M., Voice, A.K, Kalghatgi, G.T. & Babiker, H. 2016. Flammability and volatility attributes of binary mixtures of some practical multi-component fuels. *Fuel* **172**, 273–283.

Alqaheem, S.S. & Riazi, M.R. 2017. Flash Points of Hydrocarbons and Petroleum Products: Prediction and Evaluation of Methods. *Energy Fuels* **31**(4), 3578–3584.

ASTM D86-12. Standard Test Method for Distillation of Petroleum Products at Atmospheric Pressure, West Conshohocken, PA: ASTM International, 2012.ASTM D86

Baird, Z.S., Oja, V. & Järvik, O. 2015. Distribution of hydroxyl groups in Kukersite shale oil: quantitative determination by Fourier transform infrared (FTIR) spectroscopy. *Applied Spectroscopy* **68** (5), 555–562.

Baird, Z.S. & Oja, V. 2016. Predicting fuel properties using chemometrics: a review and an extension to temperature dependent physical properties by using infrared spectroscopy to predict density. *Chemometrics and Intelligent Laboratory Systems* **158**, 41–47.

Butler, R.M., Cooke, G.M., Lukk, G.G. & Jameson, B.G. 1956. Prediction of Flash Points of Middle Distillates. *Ind. Eng. Chem.* **48**, 808.

Choe, M.-H. 1988. Experimentelle und theoretische Untersuchungen zur Flammpunktbestimmung von Flüssigkeitsgemischen. Thesis.

Dyni, J.R. 2003. Geology and Resources of Some World Oil-Shale Deposits. *Oil Shale* **20**(3), 193–252.

Elenurm, A., Oja, V., Tali, E., Tearo, E. & Yanchilin, A. 2008. Thermal Processing of Dictyonema Agrillite and Kukersite Oil Shale: Transformation and Distribution of Sulfur Compounds in Pilot-Scale Galoter Process. *Oil Shale* **25**(3), 328−333.

Golubev N. 2003. Solid oil shale heat carrier technology for oil shale retorting. *Oil Shale* **20**(3), 324–332.

Gubergrits, M.J., Rohtla, I., Elenurm, A. & Myasoyedov, A.M. 1989. Comparison of light oil products from oil shale retorting in solid heat carrier units UTT-3000 and UTT-500. *Oil Shale* **6**(2), 189–194. (in Russian).

Hristova, M & Tchaoushev, S. 2006. Calculation of Flash Points and Flammability Limits of Substances and Mixtures. *J. Chem. Technol. Metall.* **41**(3), 291–296.

Hruljova, J., Savest, N., Oja, V. & Suuberg, M.E. 2013. Kukersite oil shale kerogen solvent swelling in binary mixtures. *Fuel* **105**, 77−82.

Hshieh, F.Y. 1997. Correlation of closed cup flash points with normal boiling points for silicone and general organic compounds. *Fire Mater*. **21**, 277−282.

Hughes, J.M., Hardy, D.R. & Beal, E.J. 1996. Flash Point Value for n-Dodecane Based on the Manual Pensky-Martens Closed Cup Method (ASTM D-93). *Energy & Fuels* **10**, 1276–1277.

Järvik, O. & Oja, V. 2017. Molecular Weight Distributions and Average Molecular Weights of Pyrolysis Oils from Oil Shales: Literature Data and Measurements by Size Exclusion Chromatography (SEC) and Atmospheric Solids Analysis Probe Mass Spectroscopy (ASAP MS) for Oils from Four Different Deposits. *Energy & Fuels* **31**(1), 328−339.

Kollerov, D.K. 1951. Physicochemical properties of oil shale and coal liquids (Fiziko-khimicheskie svojstva zhidkikh slantsevykh i kamenougol'nykh produktov). Moscow, 245 pp. (in Russian).

Li, X., Duan, P.P., Sun, K.N. & Yan, X. 2014. Prediction of the Flash Point of Binary and Ternary Straight-Chain Alkane Mixtures. *Advances in Materials Science and Engineering* **2014**, 5 pp.

Liaw, H-J., Gerbaud, V. & Chiu, C-Y. 2010. Flash Point for Ternary Partially Miscible Mixtures of Flammable Solvents. *J. Chem. Eng. Data* **55**, 134−14.

Mack, E., Boord, C.E & Barham, H.N. 1923. Calculation of Flash Points for Pure Organic Substances. *Industrial and Engineering Chemistry* 963–965.

Oja, V. & Suuberg, E.M. 1998. Measurements of the Vapor Pressures of Coal Tars Using the Nonisothermal Knudsen Effusion Method. *Energy & Fuels* **12**(6), 1313−1321.

Oja, V 2005. Characterization of tars from Estonian Kukersite oil shale based on their volatility. *Journal of Analytical and Applied Pyrolysis* **74**, 55−60.

Oja, V. 2007. Is it time to improve the status of oil shale science? *Oil Shale* **24**(2), 97−100.

Oja, V. & Suuberg, E.M. 2012. Oil Shale Processing, Chemistry and Technology. In: R. A. Mayer (Editors). *Encyclopedia of Sustainability Science and Technology* (7457−7491). Springer.

Oja, V. 2015. Examination of molecular weight distributions of primary pyrolysis oils from three different oil shales via direct pyrolysis Field Ionization Spectrometry. *Fuel* **159**, 759−765.

Oja, V. 2015a. Vaporization parameters of primary pyrolysis oil from Kukersite oil shale. *Oil Shale* **32**(2), 124−133.

Oja, V., Rooleht, R. & Baird, S.Z. 2016. Physical and thermodynamic properties of Kukersite pyrolysis shale oil: literature review. *Oil Shale* **33**(2), 184–197.

Patil, G.S. 1988. Estimation of flash point. *Fire Mater*. **12**, 127−131.

Phoon, L.Y., Mustaffa, A.A., Hashim, H. & Mat, R.A. 2014. Review of Flash Point Prediction Models for Flammable Liquid Mixtures. *Ind. Eng. Chem. Res.* **53**, 12553−12565.

Qian, J. 2010. *Oil Shale – Petroleum Alternative*. China Petrochemical Press, Beijing, 619 pp.

Riazi, M.R. & Daubert, T.E. 1987. Predicting flash point and pour points. *Hydrocarbon Process* **66**, 81−83.

Satyanarayana, K. & Kakati, M.C. 1991. Correlation of flash points. *Fire Mater*. **15**, 97−100.

Satyanarayana, K. & Rao, P.G. 1992. Improved equation to estimate flash points of organic compounds. *J. Hazard. Mater*. **32**, 81−85.

Savest, N., Oja, V., Kaevand, T. & Lille, Ü. 2007. Interaction of Estonian kukersite with organic solvents: A volumetric swelling and molecular simulation study. *Fuel* **86** (1−2), 17−21.

Siitsman, C., Kamenev, I. & Oja, V. 2014. Vapour pressure data of nicotine, anabasine and cotinine using Differential Scanning Calorimetry. *Thermochimica Acta* **595**, 35−42.

Siitsman, C. & Oja, V. 2015. Extension of the DSC method to measuring vapor pressures of narrow boiling range oil cuts. *Thermochimica Acta* **622,** 31−37.

Siitsman, C. & Oja, V. 2016. Application of a DSC based vapor pressure method for examining the extent of ideality in associating binary mixtures with narrow boiling range oil cuts as a mixture component. *Thermochimica Acta* **637**, 24−30.

Skrinska, M., Skrinsky, J., Dolnicek, P., Lukesova, P. & Marek, J. 2015. Flash-Point Prediction for Industrial Applications. In: *Proceedings − 2014 International Conference on Mathematics and Computers in Sciences and in Industry*, MCSI 2014, 86–88.

Suuberg, E.M. & Oja, V. 1997. Vapor pressures and heats of vaporization of primary coal tars, Technical Report, US Department of Energy, United States. doi:10.2172/774960. http://www.osti.gov/scitech/servlets/purl/774960.

Valenzuela, E.M., Vázquez-Román, R., Patel, S. & Mannan, S.M. 2011. Prediction models for the flash point of pure components. *Journal of Loss Prevention in the Process Industries* **24**, 753–757.

Walsh, R.E & Mortimer, J.V. 1971. New Way to Test Product Quality. *Hydrocarbon Processing* **50**(9), 153–158.

Wang, K.Q & Sun, X.Z. 2001. Correlation and calculation of the flash points of organic compounds. *Computational Applied Chemistry* **18**, 581–584.