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WP2 Task 2.1 Development and testing of small scale liquefier

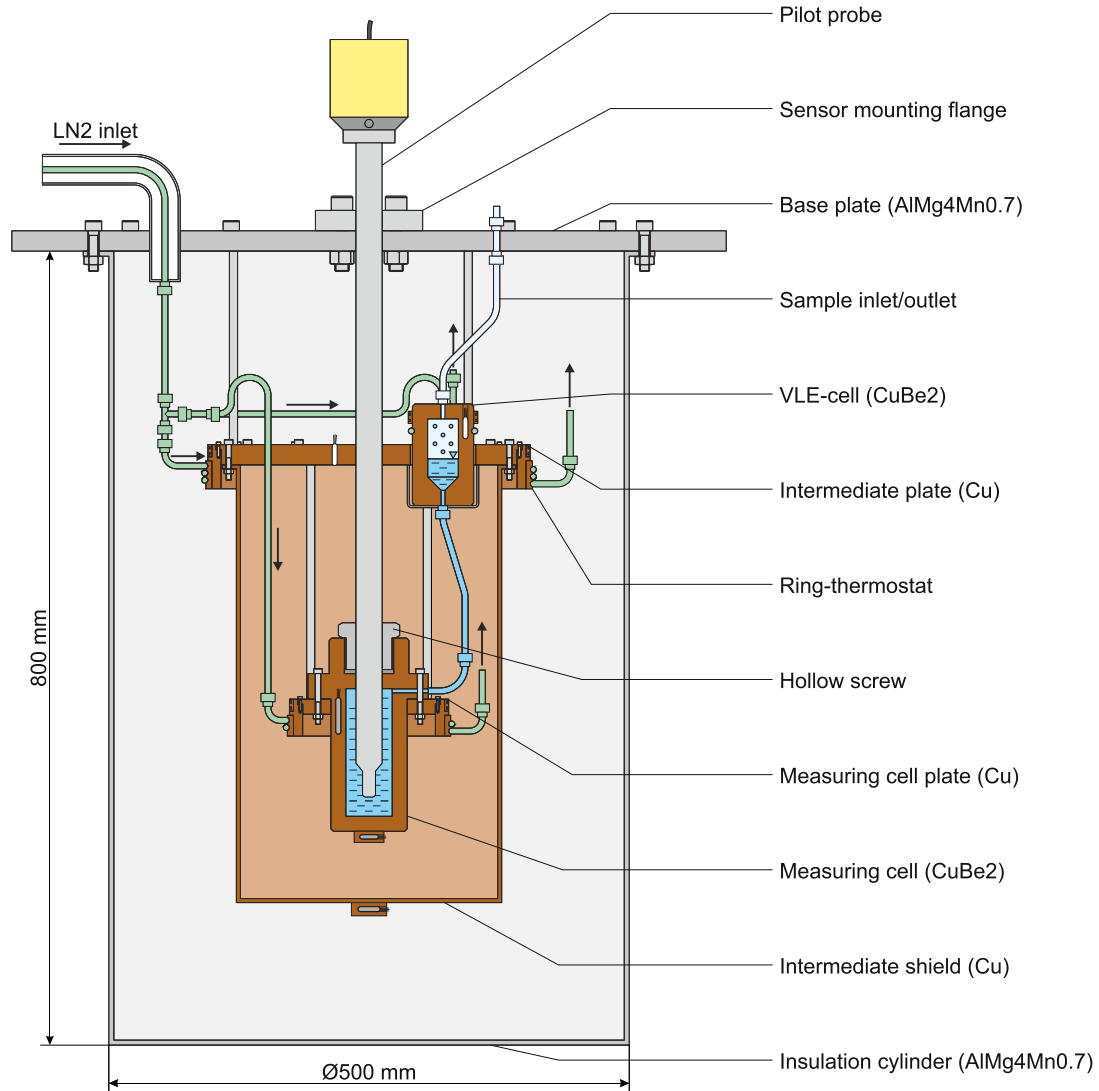
- presented at the workshop for EMPIR 16ENG09 LNG III project:
Metrological support for LNG and LBG as transport fuel

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Via Skype meeting, 28 May 2020



The design of the reference liquefier



Schematic illustration of the concept design for a small-scale reference liquefier with installed optical Raman probe

Selected 8 designed LNG-based mixtures for testing the GERG-2008 EOS

Components	Mix #1	Mix #2	Mix #3	Mix #4	Mix #5	Mix #6	Mix #7	Mix #8
Nitrogen	1.5	0.6	0.8	0.69	0.35	1.1	0.2	0.17
Methane	78.8	84.52	91.8	81.69	87.89	95.253	97.876	99.68
Ethane	14	12.9	5.7	13.38	7.27	2	1	0.09
Propane	3.4	1.5	1.3	3.67	2.92	1	0.5	0.03
iso-Butane	1.1	0.22	0.17	0.28	0.65	0.3	0.18	0.01
n-Butane	0.9	0.21	0.15	0.27	0.71	0.3	0.21	0.01
iso-Pentane	0.15	0.02	0.04	0.01	0.11	0.025	0.018	0.005
n-Pentane	0.15	0.03	0.04	0.01	0.10	0.022	0.016	0.005

Example of a flash calculation using GERG-2008 EOS by Trend 4.0

INPUT PARAMETERS				FLASH CALCULATION						
Path to EOS	D:\16ENG09 LNG III\WP2\Task 2.1\TREND				vap	liq1	liq2	sol	hyd	Overall
Input code	tp			temperature	K	150.000	150.000			150.000
Property 1	1.50E+02 K			pressure	MPa	0.900	0.900			0.900
Property 2	0.90 MPa			density	mol/m ³	849.464	22007.73			3576.591
Unit	molar			int. energy	j/mol	-6647.904	-14529.799998			-12899.083
				enthalpy	j/mol	-5588.413	-14488.905			-12647.447
				entropy	j/(mol K)	-43.266	-91.580			-81.584
Fluids	mole fractions	Eq. Type	Mix. Rules	gibbs energy	j/mol	901.489	-751.961			-409.872
nitrogen	3.50000E-03	1	1	helmholtz energy	j/mol	-158.003	-792.855			-661.508
methane	8.78900E-01	1		isob. heat capacity	j/(mol K)	43.272	62.761			-6666.000
ethane	7.27000E-02	1		isoch. heat capacity	j/(mol K)	27.586	34.136			-6666.000
propane	2.92E-02	1		speed of sound	m/s	290.764	1087.312			-6666.000
isobutan	6.50E-03	1		hydration number	-					
butane	7.10E-03	1		hydrate structure	-					
ipentane	0.0011	1		overall small cage occup	-					
pentane	0.001	1		overall large cage occup	-					
				molecular weight	kg/mol	0.016	0.019			0.019
				phase fraction	mol/mol	0.206893942	0.793106058			
				x1	mol/mol	0.012301	0.001204			nitrogen
				x2	mol/mol	0.985518	0.851087054			methane
				x3	mol/mol	0.002127	0.09111009			ethane
				x4	mol/mol	0.000052	0.036804			propane
				x5	mol/mol	0.000001	0.008195			isobutan
				x6	mol/mol	0.000001	0.008952			butane
				x7	mol/mol	0.000000	0.001387			ipentane
				x8	mol/mol	0.000000	0.001261			pentane

Flash calculation of mixture nr. 5 at 150 K, 0.90 MPa.

Sensitivity to temperature

INPUT PARAMETERS				FLASH CALCULATION						
Path to EOS	D:\16ENG09 LNG III\WP2\Task 2.1\TREND				vap	liq1	liq2	sol	hyd	Overall
				temperature	K	149.000		149.000		149.000
Input code	tp			pressure	MPa	0.900		0.900		0.900
Property 1	1.49E+02	K		density	mol/m ³	856.431		22201.28		15080.452
Property 2	0.90	MPa		int. energy	j/mol	-6663.261		-14174.161297		-14031.860
Unit	molar			enthalpy	j/mol	-5612.389		-14133.623		-13972.181
				entropy	j/(mol K)	-42.965		-91.360		-90.443
Fluids	mole fractions	Eq. Type	Mix. Rules	gibbs energy	j/mol	789.413		-520.992		-496.165
nitrogen	3.50000E-03	1	1	helmholtz energy	j/mol	-261.460		-561.530		-555.845
methane	8.78900E-01	1		isob. heat capacity	j/(mol K)	43.517		62.541		-6666.000
ethane	7.27000E-02	1		isoch. heat capacity	j/(mol K)	27.689		33.523		-6666.000
propane	2.92E-02	1		speed of sound	m/s	287.889		1067.691		-6666.000
isobutan	6.50E-03	1		hydration number	-					
butane	7.10E-03	1		hydrate structure	-					
ipentane	0.0011	1		overall small cage occup	-					
pentane	0.001	1		overall large cage occup	-					
				molecular weight	kg/mol	0.016		0.019		0.019
				phase fraction	mol/mol	0.018945913		0.981054087		
				x1	mol/mol	0.028641		0.003014		nitrogen
				x2	mol/mol	0.969639		0.877147665		methane
				x3	mol/mol	0.001677		0.07407158		ethane
				x4	mol/mol	0.000042		0.029763		propane
				x5	mol/mol	0.000001		0.006626		isobutan
				x6	mol/mol	0.000001		0.007237		butane
				x7	mol/mol	0.000000		0.001121		ipentane
				x8	mol/mol	0.000000		0.001019		pentane

Flash calculation of mixture nr. 5 at 149 K, 0.90 MPa.

Sensitivity to pressure

INPUT PARAMETERS				FLASH CALCULATION						
Path to EOS	D:\16ENG09 LNG III\WP2\Task 2.1\TREND			vap	liq1	liq2	sol	hyd	Overall	
Input code	tp			temperature	K	150.000		150.000		150.000
Property 1	1.50E+02 K			pressure	MPa	0.800		0.800		0.800
Property 2	0.80 MPa			density	mol/m ³	739.135		21408.47		1279.924
Unit	molar			int. energy	j/mol	-6608.034		-16245.015647		-10825.425
				enthalpy	j/mol	-5525.688		-16207.647		-10200.388
				entropy	j/(mol K)	-42.166		-94.120		-64.903
Fluids	mole fractions	Eq. Type	Mix. Rules							
nitrogen	3.50000E-03	1	1	gibbs energy	j/mol	799.267		-2089.608		-464.979
methane	8.78900E-01	1		helmholtz energy	j/mol	-283.079		-2126.976		-1090.016
ethane	7.27000E-02	1		isob. heat capacity	j/(mol K)	41.480		63.726		-6666.000
propane	2.92E-02	1		isoch. heat capacity	j/(mol K)	27.130		36.732		-6666.000
isobutan	6.50E-03	1		speed of sound	m/s	294.920		1192.751		-6666.000
butane	7.10E-03	1		hydration number	-					
ipentane	0.0011	1		hydrate structure	-					
pentane	0.001	1		overall small cage occup	-					
				overall large cage occup	-					
				molecular weight	kg/mol	0.016		0.022		0.022
				phase fraction	mol/mol	0.562374319		0.437625681		
				x1	mol/mol	0.005904		0.000411		nitrogen
				x2	mol/mol	0.990554		0.735418162		methane
				x3	mol/mol	0.003466		0.16166947		ethane
				x4	mol/mol	0.000073		0.066630		propane
				x5	mol/mol	0.000002		0.014851		isobutan
				x6	mol/mol	0.000001		0.016223		butane
				x7	mol/mol	0.000000		0.002514		ipentane
				x8	mol/mol	0.000000		0.002285		pentane

Flash calculation of mixture nr. 5 at 150 K, 0.80 MPa

Experiments vs. modelling on 7 LNG-based gas mixtures

Mix-2 Component	Amount (mol/mol) (experimental)	fraction	Amount (mol/mol) (modelling)	fraction	Relative deviation (%) (Exp.-Mod.)/Mod. * 100%
Nitrogen	0.007884		0.007945		-0.7693
Methane	0.869362		0.869263		0.0114
Ethane	0.070474		0.070496		-0.0309
propane	0.030329		0.030338		-0.0309
iso-butane	0.009984		0.009987		-0.0309
butane	0.009985		0.009988		-0.0309
iso-pentane	0.000975		0.000975		-0.0309
pentane	0.001008		0.001008		-0.0309

Experimental data was obtained with Raman probe inserted into the liquid while temperature was fixed in modelling.

Experiments vs. modelling on 7 LNG-based gas mixtures

Mix-6 Component	Amount (mol/mol) (experimental)	fraction	Amount (mol/mol) (modelling)	fraction	Relative deviation (%) (Exp.-Mod.)/Mod. * 100%
Nitrogen	0.002935		0.002915		0.6882
Methane	0.927884		0.927786		0.0106
Ethane	0.045158		0.045235		-0.1703
propane	0.018241		0.018272		-0.1703
iso-butane	0.003001		0.003006		-0.1703
butane	0.002482		0.002487		-0.1703
iso-pentane	0.000200		0.000201		-0.1703
pentane	0.000098		0.000098		-0.1703

Example of uncertainty calculation for using the GERG-2008 EOS

Uncertainty propagation of designed mixture 2, at 150 K and 0.1 MPa; liquid composition (x) and gas composition (y) are expressed in amount fractions (%)

Component	x	$u(x)$	$u(x)$	y	$u(y)$	$u(y)$
nitrogen	0.00248	0.00000	0.08%	0.65884	0.00046	0.07%
methane	6.87921	0.00022	0.003%	92.16259	0.00236	0.003%
ethane	71.50818	0.02169	0.03%	7.13090	0.00229	0.03%
propane	16.26268	0.01757	0.11%	$4.68 \cdot 10^{-2}$	$5.4 \cdot 10^{-5}$	0.11%
iso-butane	2.44885	0.00344	0.14%	$5.99 \cdot 10^{-4}$	$8.5 \cdot 10^{-7}$	0.14%
butane	2.34078	0.00318	0.14%	$2.55 \cdot 10^{-4}$	$3.4 \cdot 10^{-7}$	0.13%
iso-pentane	0.22309	0.00061	0.27%	$6.34 \cdot 10^{-6}$	$1.7 \cdot 10^{-8}$	0.26%
Pentane	0.33474	0.00087	0.26%	$1.91 \cdot 10^{-6}$	$4.9 \cdot 10^{-9}$	0.26%

Conclusions

- A reference liquefier was designed;
- Thermodynamic characterization of world's first EffecTech UKAS ISO 17025 accredited liquefier using the GERG-2008 was performed;
- 8 disgned LNG-based gas mixtures were used to test the GERG-2008 EOS model (using Trend 4.0);
- Experimental results performed with the EffecTech liquefier were compared with modelling on 7 LNG-based reference gas mixtures;
- A comprehensive uncertainty evaluation was conducted.

Acknowledgement

- The16ENG09 LNGIII consortium partners RUB and VSL acknowledge collaborator EffecTech for the contribution to this work

