Grant agreement No. 640979

ShaleXenvironmenT

Maximizing the EU shale gas potential by minimizing its environmental footprint

H2020-LCE-2014-1
Competitive low-carbon energy

D12.1
Journal Reviews

WP 12 – Dissemination

Due date of deliverable	28/02/2018 (Month 30)
Actual submission date	28/02/2018
Start date of project	September 1st 2015
Duration	36 months
Lead beneficiary	NCSR'D
Last editor	Evghenia Scripnic
Contributors	All partners
Dissemination level	Public (PU)

This Project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 640979.

Disclaimer

The content of this deliverable does not reflect the official opinion of the European Union. Responsibility for the information and views expressed herein lies entirely with the author(s).

History of the changes

Version	Date	Released by	Comments
0.1	22-02-2018	Evghenia Scripnic	First draft
1.0	28-02-2018	Evghenia Scripnic	Update following partners' review

Introduction

In the frame of ShaleXenvironmenT project the members of the consortium have been actively disseminating the results of the project by participating in international conferences and publishing in major scientific peer-reviewed journals. 30 months into the project, 38 papers have been accepted and published, and a number of other papers with the final results are in preparation. The table below summarises the publications for M1-M30.

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
1.	Desalination of shale gas flowback water: a rigorous design approach for zero-liquid discharge evaporation systems	V.C. Onishi, A. Carrero-Parreño, J.A. Reyes-Labarta, E.S. Fraga, J.A. Caballero	*Journal of Cleaner Production*	2017	1399-1414	10.1016/j.jclepro.2016.10.012
2.	Shale Gas Flowback Water Desalination: Single vs Multiple-effect evaporation with Vapor Recompression Cycle and Thermal Integration	V.C. Onishi, A. Carrero-Parreño, J.A. Reyes-Labarta, R. Ruiz-Femenia, R. Salcedo-Díaz, E.S. Fraga, J.A. Caballero	*Desalination*	2017	230-248	10.1016/j.desal.2016.11.003
3.	Optimal Pretreatment System of Flowback Water from Shale Gas Production	A. Carrero-Parreño, V.C. Onishi, R. Salcedo-Díaz, R. Ruiz-Femenia, E.S. Fraga, J.A. Caballero, J.A. Reyes-Labarta	*Industrial & Engineering Chemistry Research*	2017	4386-4398	10.1021/acs.iecr.6b04016
4.	Confined Water Determines Transport Properties of Guest Molecules in Narrow Pores.	PHAN Anh, COLE David R., WEIß R. Gregor, DZUBIELLA Joachim, STRIOLO Alberto.	*ACS Nano, 10*	2016	7646−7656	10.1021/acsnano.6b02942
5.	Interfacial water studies and their relevance for the energy sector	STRIOLO Alberto	*Molecular Physics, 114:18*	2016	2615-2626	10.1080/00268976.2016.1237685
6.	Molecular simulation of shale gas adsorption onto overmature type II model kerogen with control microporosity	Lukas Michalec, Martin Lisal	*Molecular Physics*	2017	1086-1103	10.1080/00268976.2016.1243739
7.	Shale gas: a life-cycle perspective for UK production	Carla Tagliaferri, Roland Clift, Paola Lettieri, Chris Chapman	*The International Journal of Life Cycle Assessment*	2016	1-19	10.1007/s11367-016-1207-5
8.	Synchrotron tomographic quantification of strain and	Fernando Figueroa Pilz, Patrick J. Dowey, Anne-	*Journal of Geophysical*	2017	2553-2564	10.1002/2016JB013874

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
	fracture during simulated thermal maturation of an organic-rich shale, UK Kimmeridge Clay	Laure Fauchille, Loic Courtois, Brian Bay, Lin Ma, Kevin G. Taylor, Julian Mecklenburgh, Peter D. Lee	*Research: Solid Earth*			
9.	Process optimization for zero-liquid discharge desalination of shale gas flowback water under uncertainty	Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Alba Carrero-Parreño, Juan A. Reyes-Labarta, Eric S. Fraga, José A. Caballero	*Journal of Cleaner Production*	2017	1219-1238	10.1016/j.jclepro.2017.06.243
10.	Modeling of Bulk Kerogen Porosity: Methods for Control and Characterization	Manolis Vasileiadis, Loukas D. Peristeras, Konstantinos D. Papavasileiou, Ioannis G. Economou	*Energy Fuels*	2017	6004– 6018	10.1021/acs.energyfuels.7b00626
11.	Transport Mechanism of Guest Methane in Water-Filled Nanopores	Tai Bui, Anh Phan, David R. Cole, and Alberto Striolo	*The Journal of Physical Chemistry*	2017	15675−15686	10.1021/acs.jpcc.7b02713
12.	Understanding Shale Gas: Recent Progress and Remaining Challenges	Alberto Striolo, David R. Cole	*Energy Fuels*	2017	10300−10310	10.1021/acs.energyfuels.7b01023
13.	A kinetic Monte Carlo approach to study fluid transport in pore networks	M. Apostolopoulou, R. Day, R. Hull, M. Stamatakis, and A. Striolo	*The Journal of Chemical Physics*	2017	134703	10.1063/1.4985885
14.	Creep of Posidonia Shale at Elevated Pressure and Temperature	E. Rybacki, J. Herrmann, R. Wirth, G. Dresen	*Rock Mechanics and Rock Engineering*	2017	-	10.1007/s00603-017-1295-y
15.	Synchrotron tomographic quantification of strain and fracture during simulated	Fernando Figueroa Pilz, Patrick J. Dowey, Anne-Laure Fauchille, Loic	*Journal of Geophysical Research: Solid Earth*	2017	2553 –2564	10.1002/2016JB013874

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
	thermal maturation of an organic-rich shale, UK Kimmeridge Clay	Courtois, Brian Bay, Lin Ma, Kevin G. Taylor, Julian Mecklenburgh, and Peter D. Lee				
16.	Adsorption and Diffusion of C1 to C4 Alkanes in Dual-Porosity Zeolites by Molecular Simulations	E Rezlerová, A. Zukal, J. Čejka, F. R. Siperstein, J. K. Brennan, M. Lísal	*Langmuir*	2017	11126-11137	10.1021/acs.langmuir.7b01772
17.	Propane−Water Mixtures Confined within Cylindrical Silica Nanopores: Structural and Dynamical Properties Probed by Molecular Dynamics	Tran Thi Bao Le and Alberto Striolo	*Langmuir*	2017	11310-11320	10.1021/acs.langmuir.7b03093
18.	EU and Regulation of Shale Industry: Where Do We Stand Now?	Jędrzej Górski, Christine Trenorden	*Oil and Gas Law News, International Bar Association*	2017	20-25	
19.	Specific ion effect on polysaccharide dispersions	Duccio Tatini, Filippo Sarri, Piefrancesco Maltoni, Moira Ambrosi, Emiliano Carretti, Barry W. Ninhama, Pierandrea Lo Nostro	Carbohydrate Polymers	2017	344-352	10.1016/j.carbpol.2017.05.078
20.	An enhanced understanding of the Basinal Bowland shale in Lancashire (UK), through microtextural and mineralogical observations	Fauchille, A-L., Ma, L., Rutter, E., Chandler, M., Taylor, K.G., Lee., P.D.	*Marine and Petroleum Geology*	2017	1374-1390	10.1016/j.marpetgeo.2017.07.030
21.	Multi-scale 3D characterisation of porosity and organic matter in shales with variable TOC	Ma, L., Taylor, K.G., Dowey, P.J., Courtois, L., Gholinia, A., Lee, P.D.	*International Journal of Coal Geology*	2017	100-112	10.1016/j.coal.2017.08.002

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
	content and thermal maturity: Examples from the Lublin and Baltic Basins, Poland and Lithuania					
22.	Shale gas flowback water desalination: multistage membrane distillation considering different configurations and heat integration	Alba Carrero-Parreño, Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, José A. Caballero, Juan A. Reyes-Labarta	*3rd International Conference on Desalination using Membrane technologies. MEMDES 2017*	2017		
23.	Quantifying the anisotropy and tortuosity of permeable pathways in clay-rich mudstones using models based on X-ray tomography	N.R. Backeberg, F. Iacoviello, M. Rittner, T.M. Mitchell, A.P. Jones, R. Day, J. Wheeler, P.R. Shearing, P. Vermeesch, A. Striolo	*Scientific Reports 7*	2017	14838	10.1038/s41598-017-14810-1
24.	Expansion of the ADOR Strategy for the Synthesis of Zeolites: The Synthesis of IPC-12 from Zeolite UOV	Valeryia Kasneryk, Mariya Shamzhy, Maksym Opanasenko, Paul S. Wheatley, Samuel A. Morris, Samantha E. Russell, Alvaro Mayoral, Michal Trachta, Jiri Cejka, and Russell E. Morris	*Angewandte Chemie*	2017	4388–4391	10.1002/ange.201700590
25.	Modelling aqueous solubility of sodium chloride in clays at thermodynamic conditions of hydraulic fracturing by molecular simulations	Filip Moucka, Martin Svoboda, Martin Lisal	*Physical Chemistry Chemical Physics*	2017	16586-16599	10.1039/c7cp02121f
26.	The Carbon-Water Interface: Perspectives on the Water-	A. Striolo, A. Michaelides, L. Joly	*Annual Review of Chemical and*	2016	533-556	10.1146/annurev-chembioeng-080615-

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
	Energy Nexus		*Biomolecular Engineering*			034455
27.	Zero-Liquid Discharge Desalination of Hypersaline Shale Gas Wastewater: Challenges and Future Directions	Viviani C. Onishi, Juan A. Reyes-Labarta, José A. Caballero	*1st Euro-Mediterranean Conference for Environmental Integration (EMCEI)*	2017	65-67	10.1007/978-3-319-70548-4_24
28.	Combining Forward and Reverse Osmosis for Shale Gas Wastewater Treatment to Minimize Cost and Freshwater Consumption	Raquel Salcedo-Díaz, Rubén Ruiz-Femenia, Alba Carrero-Parreño, Viviani C. Onishi, Juan A. Reyes-Labarta, José A. Caballero	*Computer-Aided Chemical Engineering-Elsevier Science. European Symposium on Computer Aided Process Engineering-27 (Proceedings)*	2017	2725-2730	10.1016/B978-0-444-63965-3.50456-6
29.	Optimal Shale Gas Flowback Water Desalination under Correlated Data Uncertainty	Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Alba Carrero-Parreño, Juan A. Reyes-Labarta, José A. Caballero	*Computer-Aided Chemical Engineering-Elsevier Science. European Symposium on Computer Aided Process Engineering-27 (Proceedings)*	2017	943-948	10.1016/B978-0-444-63965-3.50159-8
30.	Multistage Membrane Distillation for the Treatment of Shale Gas Flowback Water: Multi-Objective Optimization under Uncertainty	Alba Carrero-Parreño, Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, José A. Caballero, Juan A. Reyes-Labarta	*Computer-Aided Chemical Engineering-Elsevier Science. European Symposium on Computer Aided Process Engineering-27 (Proceedings)*	2017	571-576	10.1016/B978-0-444-63965-3.50097-0

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
31.	Multi-Objective Optimization of Renewable Energy-Driven Desalination Systems	Viviani C. Onishi, Rubén Ruiz-Femenia, Raquel Salcedo-Díaz, Alba Carrero-Parreño, Juan A. Reyes-Labarta, José A. Caballero	*Computer-Aided Chemical Engineering-Elsevier Science. European Symposium on Computer Aided Process Engineering-27 (Proceedings)*	2017	499-504	10.1016/B978-0-444-63965-3.50085-4
32.	Desalination of Shale Gas Wastewater: Thermal and Membrane Applications for Zero-Liquid Discharge	Viviani C. Onishi, Juan A. Reyes-Labarta, José A. Caballero	*In book: Emerging Technologies for Sustainable Desalination HandbookEdition: 1st Edition Chapter: 12*	2018		10.1016/B978-0-12-815818-0.00012-6
33.	Membrane Desalination in Shale Gas Industry. Applications and Perspectives	Viviani C. Onishi, Eric S. Fraga, Juan A. Reyes-Labarta, José A. Caballero	*In book: Emerging Technologies for Sustainable Desalination HandbookEdition: 1st Edition Chapter: 12*	2018		
34.	Transport properties of shale gas in relation to kerogen porosity	M. Vasileiadis, L.D. Peristeras, K.D. Papavasileiou, and I. G. Economou	*Journal of Physical Chemistry C*	2018		10.1021/acs.jpcc.8b00162
35.	Multi-scale models for the prediction of structure and physical properties of chemical systems related to natural gas	K.D. Papavasileiou, M. Vasileiadis, V.K. Michalis, L.D. Peristeras, and I. G. Economou	*Book chapter in Natural Gas Processing from Midstream to*	2018		

Nº	Title of the publication	Author	Journal	Year of publication	Relevant pages	DOI
	technology		*Downstream, N. Elbashir, K.R. Hall, I.G. Economou and M.M. El-Halwagi, Editors*			
36.	Variability in spatial distribution of mineral phases in the Lower Bowland Shale, UK, from the mm- to µm-scale: quantitative characterization and modelling	Fauchille, A.L., van den Eijnden, A.P., Ma L., Chandler, M., Taylor, K.G., Madi, K. Lee, P.D, Rutter, E.	*Marine and Petroleum Geology*	2018		10.1016/j.marpetgeo.2018.02.029
37.	Clay swelling in dry supercritical carbon dioxide: Effects of interlayer cations on the structure, dynamics, and energetics of CO2 intercalation probed by XRD, NMR and GCMD simulations	Loganathan, N., Bowers, G. M., Yazaydin, A. O., Schaef, H. T., Loring, J., Kalinichev, A. G., Kirkpatrick, R. J.	*Journal of Physical Chemistry C*	2018		10.1021/acs.jpcc.7b12270
38.	Concentrated aqueous sodium chloride solution in clays at thermodynamic conditions of hydraulic fracturing: Insight from molecular dynamics simulations	M. Svoboda, M. Lisal	*American Institute of Physics*	2018	222806	10.1063/1.5017166