

Supplementary material to

INTEGRATED NEURAL NETWORK AND ASPEN PLUS MODEL FOR ENTRAINED FLOW GASIFICATION KINETICS INVESTIGATION

Dario Balaban^{1,2*}, Jelena Lubura¹, Predrag Kojić¹

¹University of Novi Sad, Faculty of Technology Novi Sad, Bulevar cara Lazara 1, 21000 Novi Sad, Serbia

²University of East Sarajevo, Faculty of Technology Zvornik, Karakaj 34A, 75400 Zvornik, Republic of Srpska, Bosnia and Herzegovina

Chem. Ind. Chem. Eng. Q. 31 (3) 239–248 (2025)

Table S1. Moisture content, dry-basis (db) elemental composition (%) and LHV (MJ/kg) of feedstock materials used in this study.

Reference	Moisture	Ash _{db}	C _{db}	H _{db}	N _{db}	Cl _{db}	S _{db}	O _{db}	LHV
[1]	39.31	34.65	38.24	5.40	0.76	0.00	0.15	20.79	8.24 _{wb}
[1]	43.03	65.01	19.52	2.83	0.59	0.00	0.14	11.91	3.01 _{wb}
[1]	53.05	27.95	41.00	5.74	1.07	0.00	0.16	24.09	6.06 _{wb}
[1]	53.50	46.82	30.05	4.23	0.93	0.00	0.17	17.80	4.33 _{wb}
[1]	51.56	54.71	25.33	3.61	0.82	0.00	0.19	15.34	3.57 _{wb}
[1]	47.20	40.47	38.29	5.48	0.70	0.00	0.15	14.92	6.73 _{wb}
[1]	39.19	20.56	44.57	6.07	1.22	0.00	0.26	27.33	9.44 _{wb}
[1]	43.70	37.50	34.56	4.35	0.87	0.63	0.17	21.92	4.20 _{wb}
[1]	49.09	54.94	25.05	3.59	0.77	0.00	0.16	15.49	3.94 _{wb}
[1]	51.49	36.91	36.59	5.07	0.97	0.00	0.21	20.25	5.83 _{wb}
[1]	51.91	42.87	34.00	4.80	0.94	0.00	0.17	17.21	5.44 _{wb}
[1]	51.58	35.05	38.13	5.41	0.89	0.00	0.16	20.36	6.34 _{wb}
[1]	42.36	62.96	21.62	3.19	0.59	0.00	0.12	11.52	4.20 _{wb}
[1]	58.87	27.26	43.03	5.96	1.09	0.00	0.20	22.46	5.76 _{wb}
[1]	40.94	40.20	35.29	5.01	0.78	0.00	0.17	18.54	7.40 _{wb}
[1]	49.91	21.24	45.09	6.19	1.09	0.00	0.24	26.14	7.75 _{wb}
[1]	47.67	53.22	26.92	3.80	0.69	0.00	0.15	15.22	4.47 _{wb}
[1]	53.51	38.08	34.83	4.90	0.86	0.00	0.17	21.16	5.19 _{wb}
[1]	51.37	53.21	26.75	4.12	0.74	0.00	0.15	15.33	4.01 _{wb}
[1]	55.99	52.78	26.00	3.66	0.97	0.00	0.27	16.31	2.86 _{wb}
[1]	24.95	76.76	12.84	1.96	0.29	0.00	0.12	8.03	3.36 _{wb}
[2]	51.87	30.81	40.44	4.75	0.94	0.21	1.72	21.13	11.61 _{db}
[3]	48.00	46.15	30.77	4.62	0.77	0.00	0.39	17.30	9.95 _{db}
[4]	20.00	9.51	43.71	7.73	1.95	0.00	0.40	37.66	16.01 _{db}
[5]	44.00	30.82	37.36	5.21	0.95	0.21	0.18	25.27	6.80 _{db}
[6]	7.56	17.80	49.03	5.24	1.23	0.00	0.30	26.40	16.42 _{db}
[7]	6.30	12.40	51.60	6.30	0.80	0.00	0.20	28.70	20.17 _{db}
[8]	14.90	22.44	48.65	6.70	1.41	0.00	0.24	20.56	19.99 _{db}
[9]	57.90	10.11	47.65	6.21	2.38	0.22	0.31	33.12	3.90 _{wb}

* Email: dario.balaban@uns.ac.rs

Table S1. Continued.

Reference	Moisture	Ash _{db}	C _{db}	H _{db}	N _{db}	Cl _{db}	S _{db}	O _{db}	LHV
[9]	51.33	9.61	48.49	6.35	2.15	0.24	0.29	32.87	6.00 _{wb}
[9]	37.92	8.35	50.44	6.45	1.29	0.08	0.24	33.14	10.21 _{wb}
[9]	32.95	8.43	51.32	6.84	1.35	0.14	0.24	31.68	12.06 _{wb}
[9]	26.61	7.60	50.80	6.87	1.73	0.62	0.32	32.06	13.71 _{wb}
[10]	51.87	30.81	40.44	4.75	0.94	0.21	1.72	21.13	14.01 _{db}
[11]	25.49	33.15	36.38	4.56	1.88	0.00	0.41	23.62	12.88 _{db}
[12]	50.00	5.16	48.27	6.16	2.56	1.24	0.28	36.33	18.61 _{db}
[13]	46.54	16.52	44.43	5.73	1.60	0.00	0.22	31.50	7.74 _{wb}
[14]	51.70	46.70	29.53	1.45	1.04	0.00	0.75	20.54	9.70 _{db}
[15]	61.26	14.03	43.21	6.22	2.13	1.09	0.22	33.10	6.92 _{wb}
[16]	48.00	34.61	34.62	4.87	1.29	0.67	0.31	23.63	11.46 _{db}
[17]	81.12	0.90	44.26	6.19	1.38	0.00	0.41	46.86	16.46 _{db}
[17]	57.25	7.16	48.59	6.43	2.58	0.00	0.46	34.78	18.02 _{db}
[17]	60.34	1.70	46.72	5.95	0.00	0.00	0.32	45.31	16.24 _{db}
[17]	67.81	9.60	41.26	5.62	0.78	0.00	0.39	42.35	13.97 _{db}
[17]	71.03	5.24	43.90	6.31	1.55	0.00	0.37	42.63	15.15 _{db}
[17]	55.86	3.98	43.80	5.81	0.39	0.00	0.35	45.67	15.62 _{db}
[17]	64.58	4.71	45.04	6.07	3.47	0.00	0.50	40.21	16.96 _{db}
[17]	46.46	7.19	42.02	5.58	1.25	0.00	0.43	43.53	14.19 _{db}
[17]	47.09	15.37	37.02	5.01	2.20	0.00	0.45	39.95	12.26 _{db}
[17]	62.57	7.70	40.11	5.52	1.36	0.00	0.33	44.98	13.50 _{db}
[17]	46.87	1.71	48.07	5.99	0.05	0.00	0.39	43.79	17.33 _{db}
[17]	61.88	1.08	44.37	5.87	0.94	0.00	0.32	47.42	15.72 _{db}
[17]	69.23	5.45	43.84	6.51	1.03	0.00	0.37	42.80	15.11 _{db}
[17]	41.90	1.00	50.81	6.36	1.08	0.00	0.36	40.39	18.81 _{db}
[17]	54.27	1.02	50.34	6.26	0.00	0.00	0.31	42.07	17.54 _{db}
[17]	45.58	2.06	49.03	5.86	0.04	0.00	0.34	42.67	17.44 _{db}
[17]	62.68	4.41	43.00	5.69	2.11	0.00	0.41	44.38	15.07 _{db}
[17]	54.64	0.15	46.89	5.90	0.62	0.00	0.37	46.07	16.53 _{db}
[17]	65.70	5.72	41.33	5.90	0.39	0.00	0.34	46.32	13.90 _{db}
[17]	56.94	10.05	37.94	5.19	0.32	0.00	0.35	46.15	12.55 _{db}
[17]	58.51	3.48	47.70	5.88	0.05	0.00	0.31	42.58	16.81 _{db}
[17]	56.71	1.01	46.30	6.08	0.06	0.00	0.35	46.20	15.59 _{db}
[17]	47.68	7.31	49.03	6.40	0.94	0.00	0.42	35.90	17.87 _{db}
[17]	64.30	8.96	44.53	6.01	0.80	0.00	0.36	39.34	15.27 _{db}
[17]	63.17	0.90	48.23	6.00	0.11	0.00	0.34	44.42	17.17 _{db}
[17]	61.36	5.55	44.31	5.70	0.92	0.00	0.42	43.10	15.29 _{db}
[17]	62.93	11.05	45.28	5.89	0.94	0.00	0.42	36.42	16.01 _{db}
[17]	50.31	2.31	47.05	6.70	0.86	0.00	0.35	42.73	17.15 _{db}
[17]	60.20	4.91	42.08	5.92	0.85	0.00	0.36	45.88	13.61 _{db}
[17]	55.23	11.10	39.90	5.38	0.42	0.00	0.40	42.80	13.65 _{db}
[17]	56.81	5.36	44.78	5.75	0.49	0.00	0.40	43.22	15.62 _{db}
[17]	63.32	6.45	42.96	6.21	8.01	0.00	0.57	35.80	16.35 _{db}
[17]	54.42	8.28	45.93	6.79	6.33	0.00	0.66	32.01	18.22 _{db}
[17]	59.84	7.87	45.24	6.46	6.37	0.00	0.65	33.41	17.02 _{db}
[17]	63.20	13.06	38.97	5.45	1.79	0.00	0.42	40.31	13.57 _{db}
[17]	65.87	4.62	50.47	6.20	2.41	0.00	0.47	35.83	18.73 _{db}
[17]	75.84	1.60	48.28	5.73	0.10	0.00	0.40	43.89	16.96 _{db}
[17]	45.61	0.97	51.98	6.13	0.03	0.00	0.48	40.41	17.85 _{db}
[17]	42.21	0.72	53.30	6.69	1.57	0.00	0.39	37.33	19.45 _{db}
[18]	1.84	27.03	57.16	4.02	1.43	0.00	10.06	0.31	32.86 _{db}
[18]	1.67	12.30	74.56	4.84	1.94	0.00	4.07	2.30	33.99 _{db}
[18]	1.18	7.72	79.97	5.16	1.38	0.00	2.38	3.39	35.45 _{db}
[18]	3.38	25.02	62.41	4.45	0.95	0.00	4.16	3.01	31.75 _{db}
[18]	0.90	6.29	81.01	4.93	1.41	0.00	2.10	4.26	35.24 _{db}
[18]	5.16	33.56	51.56	3.35	1.11	0.00	6.68	3.74	30.99 _{db}
[18]	4.89	46.67	42.80	2.49	0.70	0.00	3.73	3.59	30.17 _{db}
[18]	9.31	11.71	67.80	4.77	1.68	0.00	7.42	6.62	30.89 _{db}
[18]	2.17	61.15	29.61	2.38	0.73	0.00	1.66	4.48	25.85 _{db}
[18]	16.25	9.28	69.93	4.66	1.40	0.00	1.71	13.02	30.13 _{db}
[19]	8.72	0.09	47.77	6.38	0.11	0.00	0.26	36.67	16.14 _{db}
[19]	9.80	0.79	46.63	6.49	0.09	0.00	0.36	35.84	15.95 _{db}
[19]	9.31	0.22	47.67	6.59	0.08	0.00	0.09	36.04	16.05 _{db}
[19]	9.65	0.61	46.29	6.95	0.12	0.00	0.35	36.03	15.91 _{db}
[19]	3.56	0.69	64.00	11.27	0.29	0.00	0.14	20.05	28.90 _{db}
[19]	5.73	2.19	57.00	8.90	0.07	0.00	0.28	25.83	23.45 _{db}
[19]	9.60	0.07	48.54	6.19	0.06	0.00	0.09	35.45	16.54 _{db}
[19]	8.02	3.81	45.03	6.09	0.97	0.00	0.32	35.76	15.32 _{db}
[19]	9.26	4.32	45.69	6.44	1.00	0.00	0.38	32.91	15.58 _{db}
[19]	8.20	1.12	47.40	6.28	0.33	0.00	0.28	36.39	16.35 _{db}
[19]	3.25	0.13	50.48	6.33	0.09	0.00	0.17	39.55	17.55 _{db}
[19]	3.41	0.39	62.88	9.63	1.11	0.00	0.27	22.31	27.48 _{db}
[19]	7.77	0.42	49.64	6.18	0.10	0.00	0.38	35.51	16.61 _{db}

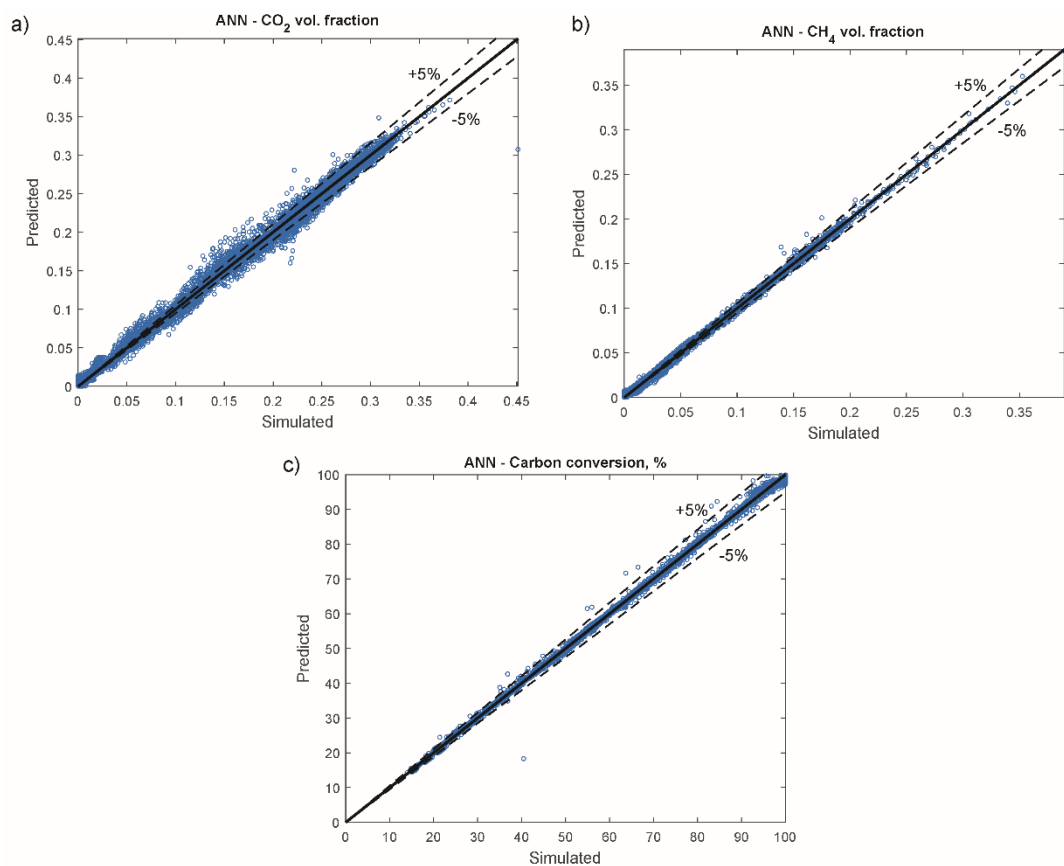


Figure S1. Simulated and predicted data on CO₂ content, CH₄ content and carbon conversion according to neural network model.

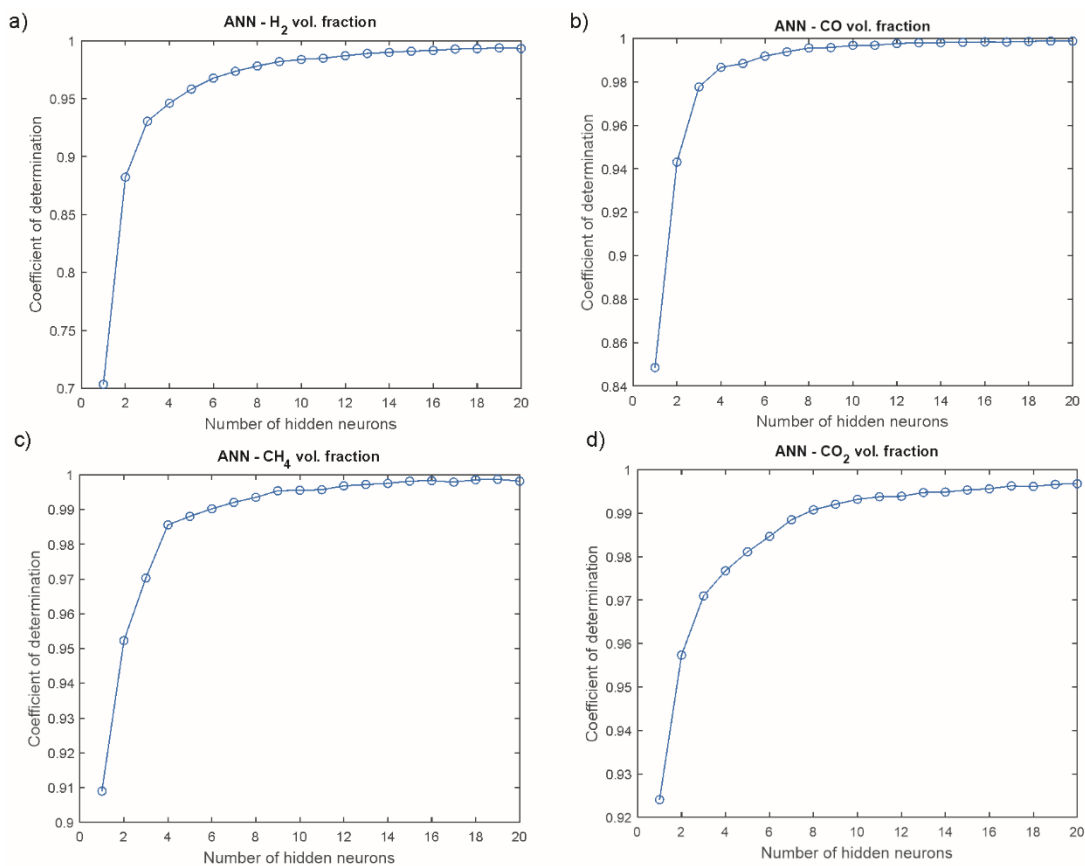


Figure S2. The impact of hidden neurons number on coefficient of determination for H₂, CO, CH₄ and CO₂ prediction via neural network.

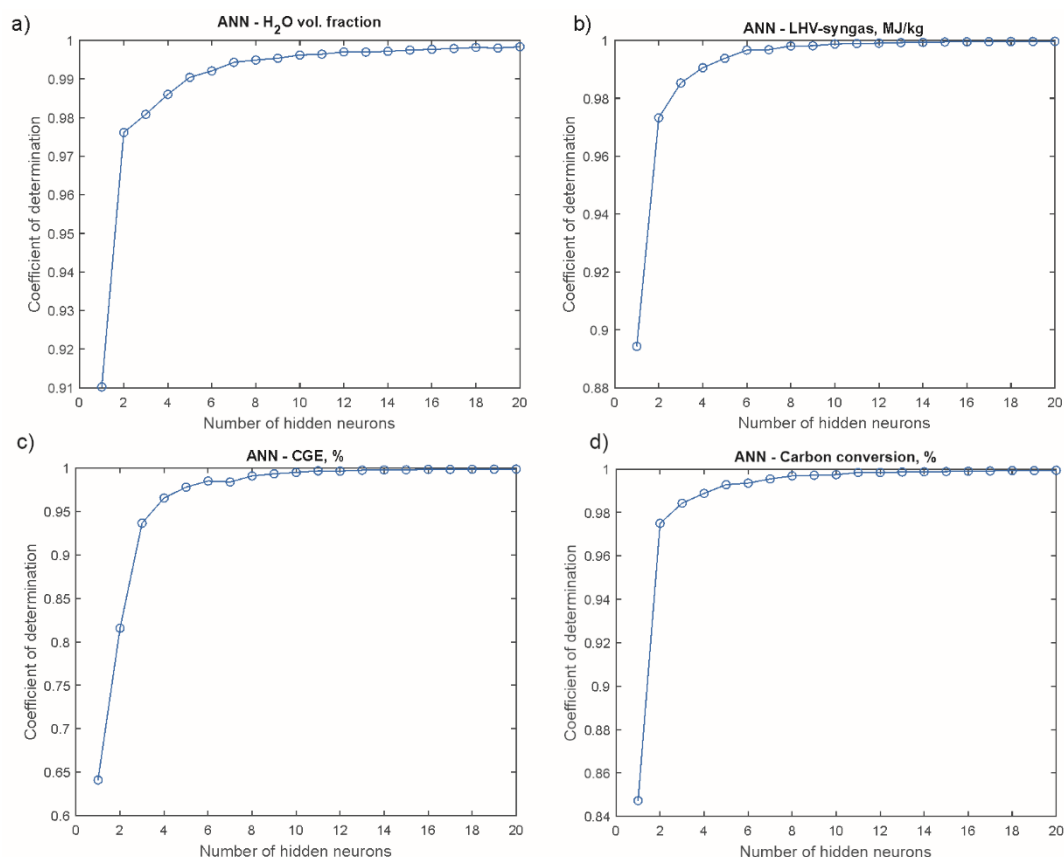


Figure S3. The impact of hidden neurons number on coefficient of determination for H_2O content, syngas LHV, CGE and carbon conversion prediction via neural network.

REFERENCES

- [1] H. Zhou, A. Meng, Y. Long, Q. Li, Y. Zhang, *Renewable Sustainable Energy Rev.* 36 (2014) 107–122. <https://doi.org/10.1016/j.rser.2014.04.024>.
- [2] M. Niu, Y. Huang, B. Jin, X. Wang, *Ind. Eng. Chem. Res.* 52 (2013) 14768–14775. <https://doi.org/10.1021/ie400026b>.
- [3] C. Chen, Y.-Q. Jin, J.-H. Yan, Y. Chi, *Fuel* 103 (2013) 58–63. <https://doi.org/10.1016/j.fuel.2011.06.075>.
- [4] A. Khuriati, P. Purwanto, H.S. Huboyo, S. Suryono, A.B. Putro, in: *J. Phys. Conf. Ser.*, IOP Publishing, 2018, p. 12006. <https://doi.org/10.1088/1742-6596/1025/1/012006>.
- [5] Y. Sun, Z. Qin, Y. Tang, T. Huang, S. Ding, X. Ma, *J. Environ. Chem. Eng.* 9 (2021) 106108. <https://doi.org/10.1016/j.jece.2021.106108>.
- [6] L. Mazzoni, M. Almazrouei, C. Ghenai, I. Janajreh, *Energy Procedia* 142 (2017) 3480–3485. <https://doi.org/10.1016/j.egypro.2017.12.233>.
- [7] S. Rudra, Y.K. Tesfagaber, *Energy* 180 (2019) 881–892. <https://doi.org/10.1016/j.energy.2019.05.125>.
- [8] P. Jiang, A.M. Parvez, Y. Meng, X. Dong, M. Xu, X. Luo, K. Shi, T. Wu, *Energy Convers. Manag.* 236 (2021) 114066. <https://doi.org/10.1016/j.enconman.2021.114066>.
- [9] N.D. Montiel-Bohórquez, A.F. Agudelo, J.F. Pérez, *Energy Convers. Manag.* 238 (2021) 114138. <https://doi.org/10.1016/j.enconman.2021.114138>.
- [10] J. Fan, H. Hong, L. Zhang, L. Li, H. Jin, *Waste Manage.* 67 (2017) 163–170. <https://doi.org/10.1016/j.wasman.2017.05.031>.
- [11] P. Sahu, V. Prabu, *Energy* 233 (2021) 121053. <https://doi.org/10.1016/j.energy.2021.121053>.
- [12] C. Chaisanguan, S. Patumsawad, P. Narataruksa, *Adv. Mat. Res. Trans. Tech. Publ.* (2013) 1270–1276. <https://doi.org/10.4028/www.scientific.net/AMR.807-809.1270>.
- [13] J. Lorenzo Llanes, E. Kalogirou, *Soc. Sci.* 8 (2019) 119. <https://doi.org/10.3390/socsci8040119>.
- [14] A. Shehzad, M.J.K. Bashir, S. Sethupathi, *Renewable Sustainable Energy Rev.* 60 (2016) 1302–1311. <https://doi.org/10.1016/j.rser.2016.03.042>.

- [15] S. Kerdsuwan, K. Laohalidanond, Appl. Mech. Mater. (2015) 1244–1248. <https://doi.org/10.4028/www.scientific.net/AMM.799-800.1244>.
- [16] G. Ding, B. He, Appl. Sci. 10 (2020) 1921. <https://doi.org/10.3390/app10061921>.
- [17] A. Ozyuguran, A. Akturk, S. Yaman, Fuel 214 (2018) 640–646. <https://doi.org/10.1016/j.fuel.2017.10.082>.
- [18] S.C. Chelgani, S. Mesroghli, J.C. Hower, Int J Coal Geol 83 (2010) 31–34. <https://doi.org/10.1016/j.coal.2010.03.004>.
- [19] M.M. Roy, K.W. Corscadden, Appl Energy 99 (2012) 206–212. <https://doi.org/10.1016/j.apenergy.2012.05.003>.