water

MDPI

Supplementary Materials

Combining Process Modelling and LCA to Assess the Environmental Impacts of Wastewater Treatment Innovations

Aleš Paulu [1,*], Jan Bartáček [2], Markéta Šerešová [1] and Vladimír Kočí [1]

[1] Department of Environmental Chemistry; Faculty of Environmental Technology; University of Chemistry and Technology Prague; Technická 5, 160 00 Prague, Czech Republic; Marketa.Seresova@vscht.cz (M.Š.); Vlad.Koci@vscht.cz (V.K.)

[2] Department of Water Technology and Environmental Engineering; Faculty of Environmental Technology; University of Chemistry and Technology Prague; Technická 5, 160 00 Prague, Czech Republic; jan.bartacek@vscht.cz

* Correspondence: paulua@vscht.cz

Table S1. Data inputs for mass and energy balance model.

Parameter	Value	Unit	Reference
General wastewater characteristics			
Influent COD flow	49 200.00		(PCWTP—personal communication 2016)
Influent $COD_{dissolved}$ concentration	0.30	kg/m³	(Henze and Comeau 2008)
Influent COD_{solid} concentration	0.45	kg/m³	(Henze and Comeau 2008)
Influent N_{total} flow at WWTP with influent COD of 120 000 kg/d	9500*	kg/d	(PCWTP—personal communication 2016)
$N_{total,dissolved}$ per N_{total} in influent	0.78		(Henze and Comeau 2008)
Influent P_{total} concentration	7.49	mg/l	(Andreoli et al. 2007)
Effluent P_{total} concentration	1.00	mg/l	(Andreoli et al. 2007)
Recirculation rate of internal recirculation	3.00		Arbitrarily defined
Recirculation rate of return sludge	2.00		Arbitrarily defined
COD per TOC in wastewater	3.02		(Pitter 2009)
Person Load of COD per day	0.12	kg/d	(Henze and Comeau 2008)
General sludge stream characteristics			
Primary sludge VSS	50.00	kg/m³	(PCWTP—personal communication 2016)
Return sludge VSS	5.90	kg/m³	(PCWTP—personal communication 2016)
Excess sludge VSS	6.80	kg/m³	(PCWTP—personal communication 2016)
Stabilized sludge VSS	30.00	kg/m³	(PCWTP—personal communication 2016)
Dewatered sludge VSS	350.00	kg/m³	(von Sperling and Gonçalves 2007)

Activated sludge VSS	3.87	kg/m^3	(PCWTP—personal communication 2016)
Sludge $COD_{dissolved}$ per VSS	1.480		(Foladori 2010)
Primary, return and excess sludge VSS per TSS	0.775		(von Sperling and Gonçalves 2007)
Stabilized sludge VSS per TSS	0.720		(PCWTP—personal communication 2016)
Dewatered sludge VSS per TSS	0.650		(von Sperling and Gonçalves 2007)
Activated sludge VSS per TSS	0.575		(von Sperling and Gonçalves 2007)
Parameters of primary clarification process [1]			
Primary clarification efficiency on COD_{solid} removal	0.53		(Metcalf & Eddy Inc. 2002)
Primary clarification efficiency on COD removal	0.36		(Metcalf & Eddy Inc. 2002)
Primary clarification emissions of CH_4 at Kralingseveer WWTP	1.00*	kg/h**	(Daelman et al. 2012)
The share of primary clarification electricity consumption in the consumption of whole WWTP	3.70	%	(Tassou 1988)
Parameters of activated sludge process [2]			
Denitrification rate of $COD_{dissolved}$ removal per N_{NH4+}	2.40	g/g	Arbitrarily defined
Denitrification rate of COD_{solid} removal per N_{NH4+}	0.46	g/g	Arbitrarily defined
Denitrification biomass yield	0.67	g/g	(Hauduc et al., 2010)
Nitrification efficiency	0.95	g/g	Arbitrarily defined
Denitrification efficiency	0.99	g/g	Arbitrarily defined
Biomass content of N_{total}	0.083	g/g	(Hauduc et al., 2010)
Nitrification removal efficiency of COD	0.90	g/g	Arbitrarily defined
Nitrification autotrophic biomass yield	0.24	g/g	(Hauduc et al., 2010)
Nitrification heterotrophic biomass yield	0.63	g/g	(Hauduc et al., 2010)
Activated sludge process emission factor of N-N_2O per influent N_{total}	2.80	%	(Daelman et al. 2013)
Activated sludge process emissions of CH_4 at Kralingseveer WWTP	2.00*	kg/h**	(Daelman et al. 2012)
Air supply to activated sludge process electricity consumption at WWTP of 410 000 PE	2 790 495.00	kWh/y**	(Veolia—personal communication 2019)
Pumping to activated sludge process electricity consumption at WWTP of 410 000 PE	1 642 937.00	kWh/y**	(Veolia—personal communication 2019)
Mixing in activated sludge process electricity consumption at WWTP of 410 000 PE	743 820.00	kWh/y**	(Veolia—personal communication 2019)
Parameters of secondary clarification process			
Secondary clarification emissions of CO_2	0.53	kg/PE/y**	(Kosse et al. 2018)
Effluent $COD_{dissolved}$ concentration	0.020	kg/m^3	Arbitrarily defined
Effluent COD_{solid} concentration	0.002	kg/m^3	Arbitrarily defined
Effluent $N_{total,dissolved}$ concentration	0.007	kg/m^3	Arbitrarily defined
Effluent $N_{total,solid}$ concentration	0.000	kg/m^3	Arbitrarily defined
Parameters of anaerobic digestion process [3]			
Anaerobic digestion efficiency on $COD_{dissolved}$ removal in primary sludge	0.74		(Mahdy et al. 2015)

Anaerobic digestion efficiency on COD_{solid} removal in primary sludge	0.74		(Mahdy et al. 2015)
Anaerobic digestion efficiency on $COD_{dissolved}$ removal in mixed sludge	0.62		(Astals et al. 2013)
Anaerobic digestion efficiency on COD_{solid} removal in mixed sludge	0.62		(Astals et al. 2013)
Content of CH_4 in biogas	0.61		(PCWTP—personal communication 2016)
Sludge thickening electricity consumption at WWTP of 410 000 PE	1 156 433.00	kWh/y**	(Veolia—personal communication 2019)
Mixing in anaerobic digestion electricity consumption at WWTP of 410 000 PE	493 078.00	kWh/y**	(Veolia—personal communication 2019)
Parameters of cogeneration unit [4]			
Emissions of CH_4 per total CH_4 generated by cogeneration unit	1.73	%	(Liebetrau et al. 2010)
Electrical energy yield per volume of biogas	1.843	kWh/m^3	(Dohányos 1998)
Parameters of dewatering process			
Digested sludge buffer tank emissions of CH_4 at Kralingseveer WWTP	4.00*	kg/h**	(Daelman et al. 2012)
Centrifuge's emissions of CH_4 at Kralingseveer WWTP	1.00*	kg/h**	(Daelman et al. 2012)
Dewatered sludge storage tank emissions of CH_4 at Kralingseveer WWTP	2.00*	kg/h**	(Daelman et al. 2012)
Reject water $COD_{dissolved}$ concentration	0.50	kg/m^3	(Henze and Comeau 2008)
Reject water COD concentration	1.16	kg/m^3	(Henze and Comeau 2008)
Reject water $N_{total,dissolved}$ concentration	0.45	kg/m^3	(Henze and Comeau 2008)
Reject water $N_{total,solid}$ concentration	0.16	kg/m^3	Arbitrarily defined
Reject water volume	930.00	m^3/d	(PCWTP—personal communication 2016)
Dewatering electricity consumption at WWTP of 410 000 PE	2 841 863.00	kWh/y**	(Veolia—personal communication 2019)
Ventilation and odor cleaning electricity consumption at WWTP of 410 000 PE	1 572 932.00	kWh/y**	(Veolia—personal communication 2019)
Parameters of sludge disposal			
Percentual distribution of stabilized sludge used in agriculture in the Czech Republic	48.00	%	(Eurostat 2015)
Percentual distribution of stabilized sludge used for composting in the Czech Republic	35.00	%	(Eurostat 2015)
Percentual distribution of stabilized sludge disposed by landfilling in the Czech Republic	10.00	%	(Eurostat 2015)
Percentual distribution of stabilized sludge disposed by incineration in the Czech Republic	7.00	%	(Eurostat 2015)
Parameters of chemically enhanced primary treatment (CEPT) [5]			
CEPT efficiency on COD_{solid} removal	0.75		(Metcalf & Eddy Inc. 2002)
CEPT efficiency on $N_{total,dissolved}$ removal	0.17		(PCWTP—personal

			communication 2016)
CEPT efficiency on COD removal	0.55		(PCWTP—personal communication 2016)
CEPT iron (III) sulfate 40% solution dose	2 557.17	kg/d	(Veolia—personal communication 2019)
Parameters of partial nitritationanammox (PN/A) process [6]			
PN/A efficiency on COD removal	70.00	%	(Castro-Barros et al. 2015)
PN/A efficiency on $N_{total,dissolved}$ removal	93.00	%	(Castro-Barros et al. 2015)
PN/A efficiency on N_{total} removal	76.60	%	(Castro-Barros et al. 2015)
PN/A emission factor of N-N_2O per influent N_{total}	2.00	%	(Castro-Barros et al. 2015)

* Re-calculated later to suit the parameters of influent wastewater described by this study. ** Converted to daily values under the assumption that an operating day is a theoretical average WWTP´s day of continual operation with no emergencies or other unexpected events. [1] We considered same efficiency of removal for COD and N_{total}. [2] CO_2 and N_2 emissions from nitrification and denitrification were calculated from COD and N_{total} mass balances of these processes. [3] We assumed no nitrogenous compounds present in biogas. [4] Biogas yield and emissions of CO_2 were calculated from COD mass balance of this process. [5] We considered same efficiency of removal for COD_{solid} and $N_{total,solid}$. [6] Electricity consumption of activated sludge process and PN/A unit in Scenario 2 were calculated regarding the amount of influent N_{total} to these processes. CO_2 and N_2 emissions from PN/A process were calculated from COD and N_{total} mass balance of this process.

Table S2. Additional life-cycle assessment data.

Name	Notes	Reference
Electricity grid mix	Average specific electricity supply in Czech Republic including consumption, distribution, and import. The origin being 42% lignite, 32% nuclear and other.	(thinkstep 2019)
Iron (III) sulfate production	Data set covering all relevant process steps and technologies of life cycle of iron (III) sulfate	(thinkstep 2019)
Composting *	Open windrow composting plant, without collection and transport of waste but including the production of good quality compost and the utilization of compost. The plant is based on the treatment of average biodegradable waste.	(thinkstep 2019)
Landfill	Data set covering all relevant process steps and technologies for the treatment of waste on a landfill. Including landfill gas utilization and leachate treatment and without collection, transport, and pre-treatment.	(thinkstep 2019)
Incineration	Average European waste-to-energy plant, without collection, transport, and pre-treatment. The plant is based on the treatment of average European municipal solid waste.	(thinkstep 2019)

* This process was attributed to stabilized sludge, which was used for composting and in agriculture in the Czech Republic (83%), as we assumed these two disposal techniques have very similar environmental impacts.

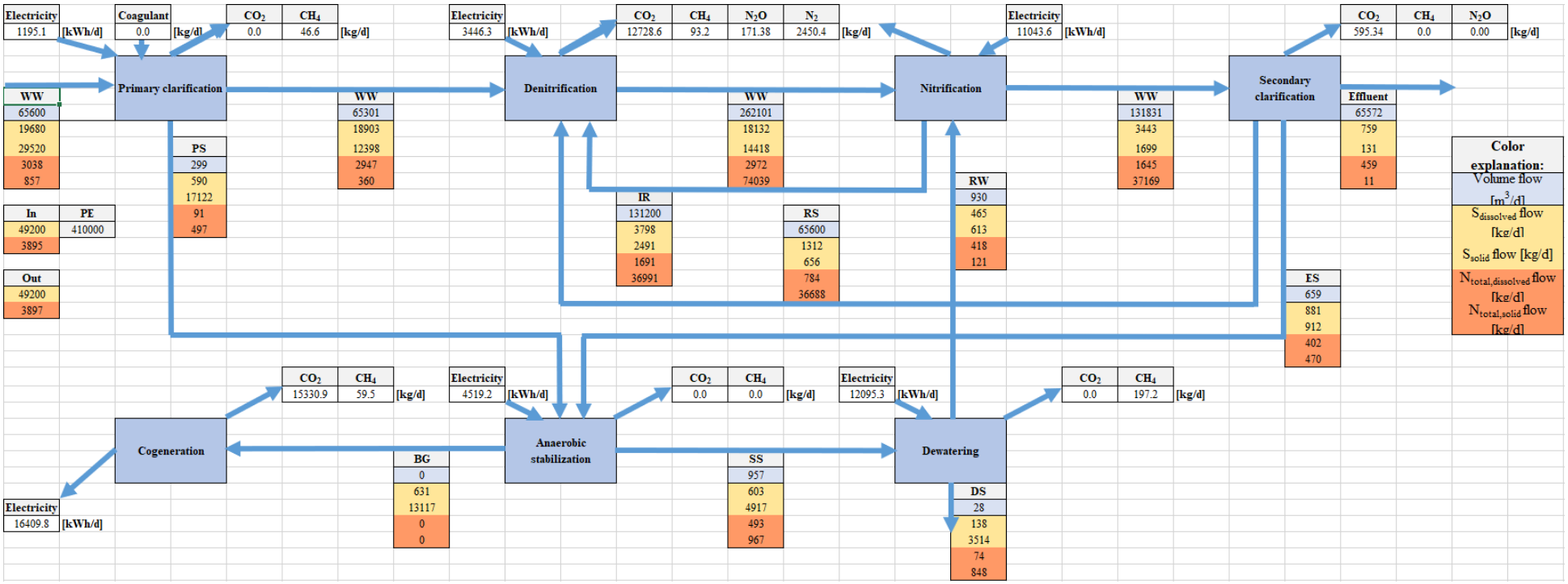

Figure S1. Screenshot of mass and energy balance model scheme for Scenario 1 in MS Excel software. WW = Wastewater, PS = Primary sludge, IR = Internal recirculation, RS = Return sludge, RW = Reject water, ES = Excess sludge, BG = Biogas, SS = Stabilized sludge, DS = Dewatered sludge.

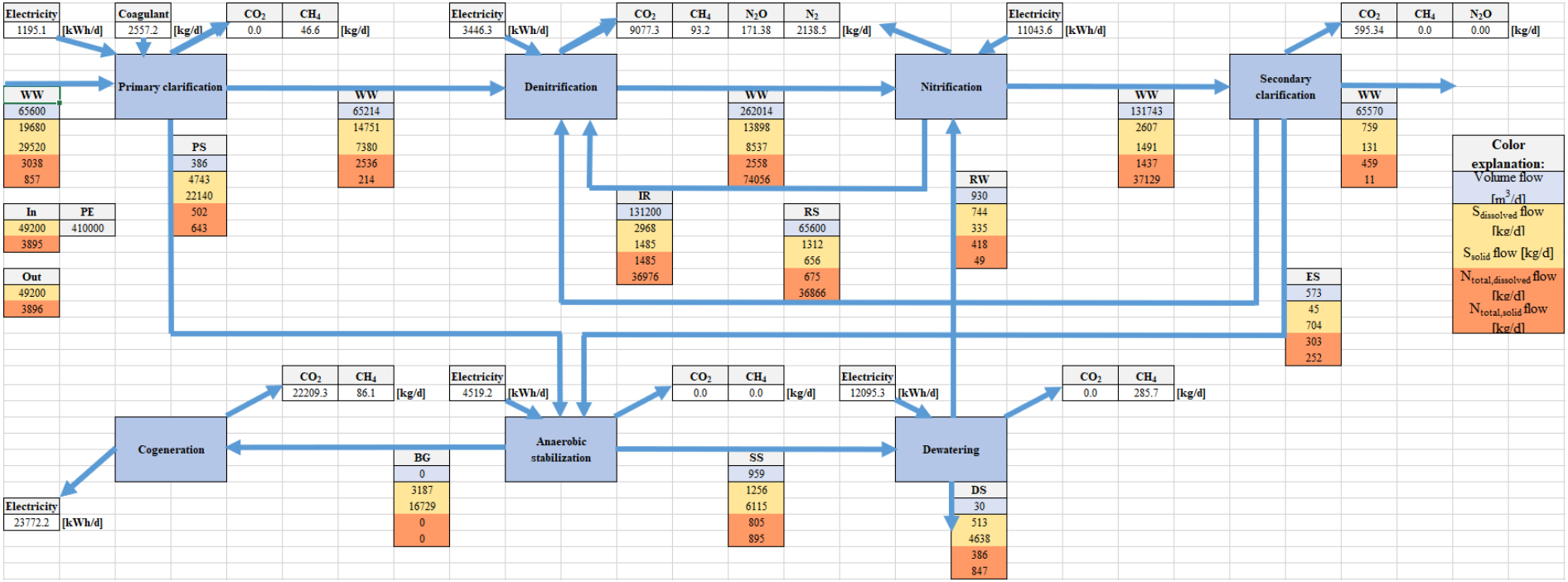

Figure S2. Screenshot of mass and energy balance model scheme for Scenario 2 in MS Excel software. WW = Wastewater, PS = Primary sludge, IR = Internal recirculation, RS = Return sludge, RW = Reject water, ES = Excess sludge, BG = Biogas, SS = Stabilized sludge, DS = Dewatered sludge.

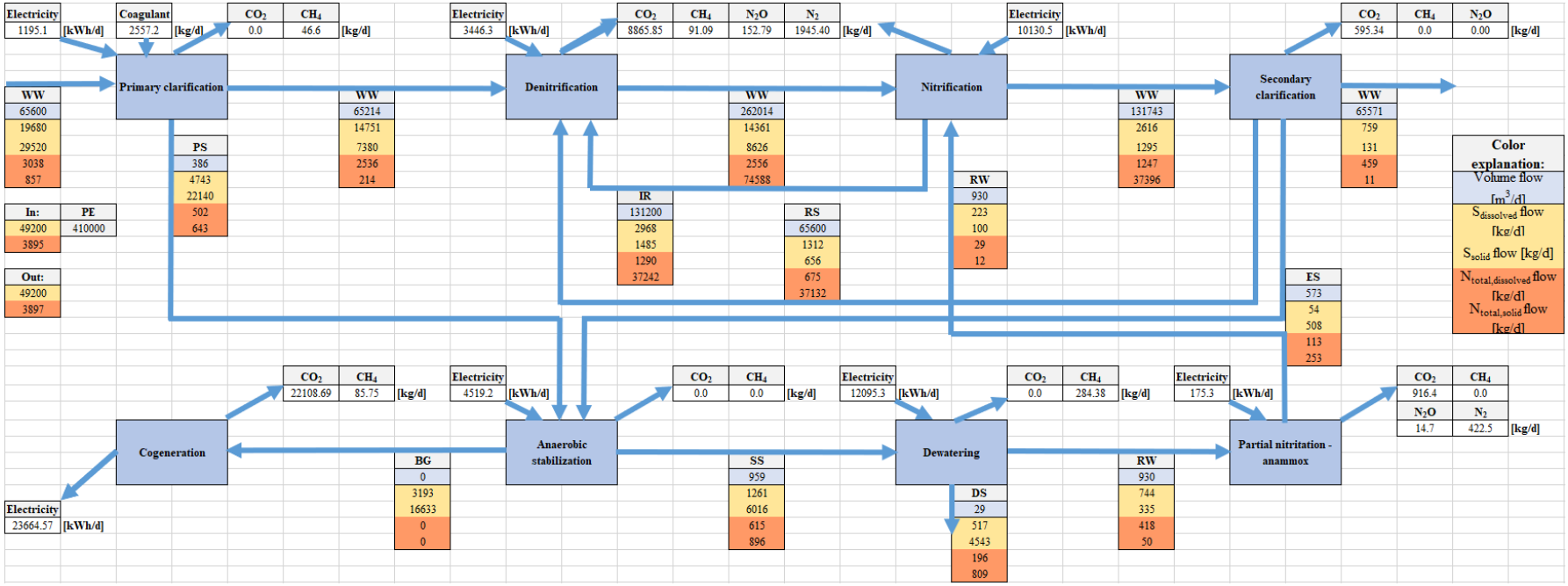

Figure S3. Screenshot of mass and energy balance model scheme for Scenario 3 in MS Excel software. WW = Wastewater, PS = Primary sludge, IR = Internal recirculation, RS = Return sludge, RW = Reject water, ES = Excess sludge, BG = Biogas, SS = Stabilized sludge, DS = Dewatered sludge.

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