A mechanistic model to assess the fate of PAHs in a Chilean WWTP and implication for effluent reuse and solids disposal

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Table S1. Influent naphthalene loads (g/d) obtained through the bootstrap for the 10%, 50% and 95% probability percentiles

	P10	P50	P95
E1	170.7	397.9	715.3
Q1	184.1	416.9	749.5
Q2	191.4	426.4	760.1
Q3	201.6	434.4	773.0
E2	221.0	454.0	795.4

Table S2. Influent benzo(a)pyrene loads (g/d) obtained through the bootstrap for the 10%, 50% and 95% probability percentiles

	P10	P50	P95
E1	4.4	24.9	82.9
Q1	5.6	27.3	83.6
Q2	6.2	28.4	84.4
Q3	9.1	32.1	84.8
E2	10.2	33.9	86.2

Details About the Mechanistic Model

Table S3. Assumptions for each treatment stage in the PAH model

Treatment stage	Compartments	Processes	Considerations	Reference
Primary treatment	Dissolved and adsorbed to MP	Advection, adsorption, surface volatilization	Equilibrium between dissolved and sorbed phase. A linear isotherm is used to characterize the process. Sorption occurs onto total suspended solids. Volatilization occurs only to the dissolved phase.	[1]
Secondary treatment	Dissolved and adsorbed to sludge	Advection, adsorption, biodegradation (oxic and anoxic conditions), surface and bubble volatilization	Equilibrium between dissolved and sorbed phase. Sorption occurs onto total suspended solids. Volatilization occurs only to the dissolved phase. Retransformable fraction is not considered. Biodegradation occurs as cometabolism.	[1,2]
Thickeners and dewatering	Freely dissolved, sorbed to particles and sorbed to DCM	Advection	No chemical or biological processes of PAHs take place. No interaction between PAH sorbed to particles and sorbed to DCM.	[3]
Anaerobic digestion	Freely dissolved, sorbed to particles, sorbed to DCM and gas	Advection, sorption/desorption to particles, sorption/desorption to DCM, volatilization, biodegradation	Biodegradation occurs as cometabolism to the bioavailable fraction (freely dissolved and sorbed to DCM). Volatilization occurs to the freely dissolved phase. No interaction between PAHs sorbed to particles and sorbed to DCM. Sorption/desorption modelled as a first order reaction.	[4]

The general ecuation for each phase considered in each treatment stage is:

$$0 = r_{adv,i} \pm r_j$$

Where, $r_{adv,i}$: Advection rate (Fin – Fout) in the i-phase; r_j: rate of j-process. The different processes for each treatment stage are presented in Table B2 and B4 for the water line and sludge line, respectively. .
The information regarding operational parameters was obtained from SISS, 2014 [39].

Table S4. Rate ecuations for the processes considered in the water line

Treatment statge	Process	C_{dis}	C_{ad}	Rate	Reference
Primary treatment	Sorption to particles	-1	+1	$Q \cdot K_{d,prim} \cdot C_{dis} \cdot X$	[1]
	Superficial volatilization	-1		$V \cdot K_L a_{sur} \cdot C_{dis} \frac{H_c}{H_c + (k_L/k_G)}$	
Secodary treatment	Sorption to particles under aerobic condition	-1	+1	$K_{d,Ox,sec} \cdot C_{LI} \cdot \frac{S_o}{K_o + S_o} \cdot X$	[1,2]

	Sorption to particles under anoxic condition	-1	+1	$K_{d,Ax,sec} \cdot C_{LI} \cdot \frac{K_o}{K_o + S_o} \cdot X$	
	Superficial volatilization	-1		$V \cdot K_L a_{sur} \cdot C_{dis} \frac{H_c}{H_c + (k_L/k_G)}$	
	Bubble volatilization	-1		$-GH_cC_{dis}\left(1 - \exp\left[-\frac{K_L a_{bub} Z}{H_c U}\right]\right)$	
	Biodegradation in oxic condition	-1		$\left[q_{C,Ox} \cdot \frac{S_s}{K_s+S_s} + k_{Bio,Ox}\right] C_{LI} \frac{S_o}{K_o+S_o} X_{SS}$	
	Biodegradation in anoxic condition	-1		$\left[q_{C,Ax} \cdot \frac{S_s}{K_s+S_s} + k_{Bio,Ox}\right] C_{LI} \frac{S_o}{K_o+S_o} X_{SS}$	

Table S5. Parameters used in the water line

Name	Parameter	Unit	Nap	B(a)p	Reference
Ratio of the liquid-phase mass transfer coefficient to the gas-phase mass transfer coefficient for surface volatilization	$(k_L/k_G)_{sur,p}$	-	0.025		[1]
Dimensionless Henry's law coefficient	H_c	-	0.03	0.0008	[5]
Linear partition coefficient for primary sludge	$K_{d,prim}$	L/kgSST	0.86	35.1	[1]
Overall surface-desorption gas-transfer coefficient	$K_{L*asur,p}$	d^{-1}	1.8		[1]
Biotransformation rate	k_{bio}	L/gSSV*d	0.11	0.013	[6]
Solid-liquid sorption coefficient for secondary sludge	$K_{d,sec}$	L/gSST	2.2	9.7	[7]
Half saturation coefficient for Ss	Ks	mgCOD/L	10		[8]
Half saturation coefficient for dissolved oxygen	Ko	mgO2/L	0.2		[8]
Aerobic maximum specific cometabolic substrate biotransformation rate in the presence of growth substrates for CLI	$q_{c,ox}$	L/g*d	2.4		[2]
Aerobic maximum specific cometabolic substrate biotransformation rate in the presence of growth substrates for CLI	$q_{c,ax}$	L/g*d	0.96		[2]
Gas flow rate	G	m^3/d	47500		[1]
Overall gas-transfer coefficient for bubble desorption	$K_{L*}a_{bub}$	d^{-1}	64700		[1]
Superficial bubble rising velocity	U	m/d	7780		[1]
Water column depth	Z	m	6		[9]

Table S6. Rate ecuations for the processes considered in the sludge line

Treatment stage	Process	C_f	C_{DCM}	C_p	C_g	Rate	Reference
Anaerobic digestion	Volatilization	-1			+1	$K_{La}(K_H \cdot C_f - C_g)$	[4]
	Sorption to particles	-1		+1		$k_1(K_p C_f - c_p)$	
	Sorption to DCM	-1	+1			$k_2(K_{DCM} C_f - c_{DCM})$	
	Biodegradation of free dissolved compartment	-1				$\left(T_c \frac{\mu}{Y} + k_c\right)\left(\frac{C_{free}}{K_{SC} + C_{free}}\right)X$	
	Biodegradation of sorbed to DCM compartment		-1			$\left(T_c \frac{\mu}{Y} + k_c\right)\left(\frac{C_{DCM}}{K_{SC} + C_{DCM}}\right)X$	

Table S7. Parameters used in the sludge line

Name	Parameter	Unit	Nap	B(a)p	Reference
Biomass maximum growth rate	μ_{max}	d^{-1}	0.62		[4]
Half saturation of growth substrate	Ks	gCOD/L	5.10		[4]
Growth yield	Y	gCOD-X/gCOD-Ss	0.75		[4]
First order endogenous decay	b	d-1	0.05		[4]
PAH transformation capacity	T_c	µgPAH/gCOD-Ss	1.90		[10]
Maximum specific rate of OMPs biodegradation in absence of primary substrate	kc	µgPAH/gCOD-X*d	0.27	0.06	[6]
Half saturation constant of PAHs	K_{SC}	µgPAH/L	7,948	30,345	[11]
First order kinetic of hydrolysis	k_{hyd}	d^{-1}	0.14		[9]
Overall surface-desorption gas-transfer coefficient	K_{La}	d^{-1}	100		[12]
Dimensionless Henry's law coefficient	K_H	-	0.03	0.00079	[5]
First order kinetic constant of sorption to particles	k_1	d^{-1}	0.0067	0.015	[13]
First order kinetic constant of sorption to DCM	k_2	d^{-1}	0.0067	0.015	[13]
Equilibrium constant for PAH sorption to particle	K_{part}	L/gCOD	1.92	12.10	[4]
Equilibrium constant for PAH sorption to DCM	K_{DCM}	L/gCOD	7.98	50.35	[4]

Results for the sensitivity analysis

Table S8. Variations in the PAH load present in the effluent for variations of ±25%, ±50%, and ±75%

Parameter	Phase	-75%	-50%	-25%	25%	50%	75%
	Fdis	1.25	1.15	1.07	0.94	0.88	0.83
	Fad	0.31	0.58	0.80	1.17	1.32	1.46
Kd, prim	Ft	1.21	1.13	1.06	0.95	0.90	0.86
	Fdis	1.25	1.15	1.07	0.94	0.88	0.83
	Fad	0.31	0.58	0.80	1.17	1.32	1.46
Kd,sec	Ft	1.21	1.13	1.06	0.95	0.90	0.86
	Fdis	1.38	1.19	1.08	0.93	0.88	0.83
	Fad	1.38	1.19	1.08	0.93	0.89	0.83
SRT	Ft	1.38	1.19	1.08	0.93	0.88	0.83
	Fdis	1.00	1.00	1.00	1.00	1.00	1.00
	Fad	1.00	1.00	1.00	1.00	1.00	1.00
k1	Ft	1.00	1.00	1.00	1.00	1.00	1.00
	Fdis	1.01	1.00	1.00	1.00	1.00	1.00
	Fad	1.01	1.00	1.00	1.00	1.00	1.00
kP	Ft	1.01	1.00	1.00	1.00	1.00	1.00

Table S9. Variations in the PAH load present in the biosolids for variations of ±25%, ±50%, and ±75%

Parameter	Phase	-75%	-50%	-25%	25%	50%	75%
	Ffree	0.75	0.84	0.93	1.07	1.14	1.20
	FDCM	1.01	1.01	1.00	1.00	0.99	0.99
	Fp	0.72	0.82	0.92	1.08	1.15	1.21
Kd, prim	Ft	0.75	0.84	0.92	1.07	1.13	1.19
	Ffree	0.70	0.82	0.91	1.09	1.16	1.20
	FDCM	0.97	0.97	0.98	1.01	1.03	1.04
	Fp	0.67	0.79	0.94	1.08	1.16	1.22
Kd,sec	Ft	0.69	0.81	0.95	1.08	1.15	1.21
	Ffree	0.6	0.8	0.9	1.1	1.1	1.2
	FDCM	1.0	1.0	1.0	1.0	1.0	1.0
	Fp	0.6	0.8	0.9	1.1	1.2	1.2
SRT	Ft	0.6	0.8	0.9	1.1	1.1	1.2
	Ffree	0.59	0.80	0.93	1.07	1.11	1.14
	FDCM	0.85	0.92	0.97	1.02	1.04	1.05
	Fp	1.02	1.01	1.00	0.99	0.99	0.99
k1	Ft	1.01	1.00	1.00	1.00	1.00	1.00
	Ffree	1.86	1.45	1.18	0.86	0.77	0.68
	FDCM	1.32	1.17	1.07	0.95	0.91	0.88
	Fp	0.96	0.98	0.99	1.01	1.01	1.02
kP	Ft	0.99	0.99	1.00	1.00	1.00	1.00

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