

SUPPORTING INFORMATION

Systematic Design, Optimization and Sustainability Assessment for Generation of Efficient Wastewater Treatment Networks

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A. Information for Municipal Case Study

A.1 Model equations and details

- a) *The uppercase italic Latin fonts (not colored) are for variables (optimization variables)*
- b) *The uppercase Latin font and lowercase Greek fonts in red are the specified input parameters*
- c) *Parameters evaluated from available inputs are the uppercase Latin fonts and lowercase Greek fonts in color green.*
- d) *The parameter or variable to be evaluated is always on the L.H.S of the equation*

A.1.1 Indices and Sets

$i \in I$ – technologies (used as subscript to variables)

<i>flc</i>	-	flocculation,
<i>sdm</i>	-	sedimentation,
<i>ftt</i>	-	filtration,
<i>ads</i>	-	adsorption,
<i>asl</i>	-	activated sludge,
<i>rbc</i>	-	rotating biological contactors,
<i>dis</i>	-	disinfection,
<i>mbrt</i>	-	membrane bioreactor,
<i>aop</i>	-	advanced oxidation process,
<i>bic</i>	-	bleaching,
<i>mbr</i>	-	membrane processes
<i>splt#</i>	-	splitter and # = {1, 2, 3, 4}

$m_{xr\#}$ - mixer and $\# = \{1, 2, 3, 4\}$
 $b_{yp\#}$ - bypass and $\# = \{1, 2, 3, 4\}$

$j \in J$ – stream (used as subscript to variables)

$\{1, 2, 3, 4, \dots, 49\}$

$k \in K$ – components (used as subscript to variables)

$\{W_{tr}$ - water,
 S_{sld} - solids,
 M_{tls} - metals
 $Chem$ - chemicals
 Fl_{cnt} - flocculants,
 Oz - ozone,
 $NaClO$ - sodium hypochlorite,
 L_{Chlrn} - liquid chlorine}

$s \in S$ - stages $\{s1, s2, s3, s4\}$

A.1.2 Subsets

Subsets for technologies

I^{CST} – technologies with costs
 $\{flc, sdm, ftt, ads, asl, rbc, mbrt, dis, mbr, blc\}$

I^{CF} – technologies with concentration factor
 $\{ftt, mbrt, sdm, mbr\}$

I^{CONS} – technologies with consumables
 $\{ftt, ads, mbrt, mbr\}$

I^{EAC} – technologies with externally added components
 $\{flc, aop, dis, blc\}$

I^{BV} – technologies with binary variables
 $\{flc, sdm, ftt, ads, asl, rbc, mbrt, dis, mbr, blc, byp1, byp2, byp3, byp4\}$

I^{S1} – technologies in stage 1
 $\{flc, byp1\}$

I^{S2} – technologies in stage 2
 $\{ftt, sdm, byp2\}$

I^{S3} – technologies in stage 3
 $\{ads, asl, rbc, dis, mbrt, byp3\}$

I^{S4} – technologies in stage 4
 $\{aop, blc, mbr, byp4\}$

Subsets for streams

J^{flc} – streams for flocculation
 $\{2, 4, 5\}$

J^{byp1} – streams for bypass 1

- $\{3, 6\}$
- J^{sdm} – streams for sedimentation
 $\{9, 13, 14\}$
- J^{flt} – streams for filtration
 $\{8, 11, 12\}$
- J^{byp2} – streams for bypass 2
 $\{10, 15\}$
- J^{ads} – streams for adsorption
 $\{17, 23, 24\}$
- J^{asl} – streams for activated sludge
 $\{18, 25, 26\}$
- J^{rbc} – streams for rotating biological containers
 $\{19, 27, 28\}$
- J^{dis} – streams for disinfection
 $\{20, 29, 30, 31\}$
- J^{mbrt} – streams for membrane bioreactor
 $\{21, 32, 33\}$
- J^{byp3} – streams for bypass 3
 $\{22, 34\}$
- J^{aop} – streams for advanced oxidation process
 $\{36, 40, 41, 42\}$
- J^{mbr} – streams for membrane processes
 $\{38, 46, 47\}$
- J^{blc} – streams for bleaching
 $\{37, 43, 44, 45\}$
- J^{byp4} – streams for bypass 4
 $\{39, 48\}$

Subsets for components

- K^{S} – components in streams
 $\{Wtr, Ssld, Mtls, Chem, Flcnt, Oz, NaClO, L_Chlrn\}$
- K^{SP} – components in initial wastewater stream
 $\{Wtr, Ssld, Mtls, Chem\}$
- K^{CONT} – components that are contaminants
 $\{Ssld, Mtls, Chem\}$
- K^{EAC} – components that are externally added
 $\{Flcnt, Oz, NaClO, L_Chlrn\}$

A.1.3 Dynamic sets for connectivity

- J_i - streams of technology i
- J_{in_i} - inlet streams of technology i

J_{out_i} - outlet streams of technology i

K_i - components k in technology i

K_j - components k in stream j

A.1.4 Model Parameters

General Parameters

ρ_k (kg/m³) = Density of component k

π_{WW} (m³ WW/h) = Entering volumetric flowrate of wastewater (WW)

π^{Rep_i} (\$/unit) = Replacement cost of consumables per unit capacity in technology i

μ (N-s/m²) = viscosity of fluid

η_i (%) = efficiency of technology i

θ_i^R (hr) – residence time in technology i

θ_i^{Rep} (h/year) = Replacement time for consumables in technology i

τ_{ann} (h/annum) = annual operation in hours (330 day x 24 h/day = 7920 hrs)

$C0_i$ (\$/capacity) = standard capacity cost in technology i

g (m/s²) = gravitational constant

nc = cost scaling index (2/3 rule)

$Nlabr_i$ (#/h) = standard # of laborers required for technology i per hour

$Q0_i$ (m³ or m² or m³/h) = standard capacity of technology i

MW_k (kg/kmol) = molecular weight of component k

Min_k (kg/m³) = initial mass concentration of component k

$Cpur_k$ (\$/kg) = purchase cost of added component k

Wsp_i (kW/h) = standard power required for technology i per hour

MM_k (--) = Big-M constant for component k

Φ_k (kg/kg WW) = amount of externally added component k

dp (m) = diameter of particle

$\xi_{j,i}$ (--) = retention factor of component k for technology i {*ftt*, *mbrt*, and *mbr* technologies}

ζ_{RF} (--) = capital recovery/ charge factor (0.11)

ζ_i (m³/m²h) = flux of technology i {*ftt*, *mbrt*, and *mbr* technologies}

κd_i (h⁻¹) = decay of biomass coefficient of technology i {*asl* technology}

γ_i (kg/kg) = biomass yield of technology i {*asl* technology}

χ_i (m³/m²h) = hydraulic loading of technology i {*rbc* technology}

BMC_{mult} (--) = bare module cost multiplier (5.4)

C_{Lab} (\$/h) = labor cost – operator basis (30)

C_{Elec} (\$/kW) = cost of electricity per hour (0.1)

Evaluated Parameters

SOR_i (m/s) = surface overflow rate id sedimentation

U_i (m/s) = settling velocity of technology i

A.1.5 Model Variables

General Variables

Cc_i (\$) = Purchase cost of technology $i \in I^{CST}$

CF_i (m³/m³) = Concentration factor for technologies $i \in I^{CF}$

Cpr_k (\$/h) = Purchase cost of added components $k \in K^{EAC}$

$M_{j,k}$ (kg/h) = Mass flowrate of component k in stream j

Qc_i (m³ or m² or m³/h) = capacity cost of technologies $i \in I^{CST}$

PW_i (kW/h) = power requirements for technologies $i \in I^{CST}$

$Nlbr_i$ (#/h) = number of laborers required for technology $i \in I^{CST}$

Yo_i (kg/kg) = observed bacteria yield of technology i (*asl* technology)

Sr_i (m/h) = settling rate of unit i (*asl* technology)

X_i (kg/h) = biomass produced in technology i (*asl* technology)

Srt_i (h) = solids residence time in technology i (*asl* technology)

D_i (m) = diameter of technology i (*mbrt* technology)

$Consi$ (\$/annum) = consumable cost of technology $i \in I^{CONS}$

Binary Variables

y_i (--) = binary variables for technologies to selected $i \in I^{BV}$

Stage-wise Costing Variables

$CCAC_{Nstg}$ = annualized capital (fixed) cost in nth stage

$CCRM_{Nstg}$ = material cost in nth stage

$CCCS_{Nstg}$ = consumable cost in nth stage

$CCLB_{Nstg}$ = labor cost in nth stage

$CCUT_{Nstg}$ = utility cost in nth stage

$CCOT_{Nstg}$ = other cost in nth stage (plant overhead and supervision costs)

$CCTC_{Nstg}$ = total cost in nth stage (all cost added in that particular stage)

$CCTPC$ = total cost for process (summation of total cost in each stage)

A.1.6 Model Equations:

Initial wastewater flowrate equations:

$$M_{1,k} = (\sum_k Min_k) \pi_{WW} ; \forall k \in K^{SP}$$

Component balances in all technologies:

$$\sum_{j \in J_{in_i}} M_{j,k} = \sum_{j \in J_{out_i}} M_{j,k} ; \forall k \in K^S$$

Cost of technologies:

$$\left(\frac{C_{c_i}}{CO_i} \right) = \left(\frac{Q_{c_i}}{QO_i} \right)^{nc} ; \forall i \in I^{CST}$$

Labor requirements in technologies:

$$Nlbr_i QO_i = Nlabr_i Qc_i ; \forall i \in I^{CST}$$

Consumable costs in technologies:

$$Cons_i = \frac{\tau_{ann}}{\theta_i^{Rep}} \pi_i^{Rep} Qc_i ; \forall i \in I^{CST}$$

Logical equations:

$$M_{i,j} - M1_{k} y_i \leq 0 ; \forall i \in I^{BV} , j \in J , k \in K_i \text{ and } K_j$$

Selection of technologies in each stage:

Preliminary (Pretreatment) stage:

$$y_{flc} + y_{byp,1} = 1$$

Primary Treatment Stage:

$$y_{ftt} + y_{sdm} + y_{byp,2} = 1$$

Secondary Treatment Stage:

$$y_{ads} + y_{asl} + y_{rbc} + y_{dis} + y_{mbrt} + y_{byp,3} = 1$$

Tertiary Treatment Stage:

$$y_{aop} + y_{mbr} + y_{blc} = 1$$

Preliminary (Pretreatment) Stage Model Equations for Technologies

Flocculation (flc):

Flocculent added:

$$M_{5,Flcnt} = \Phi_{Flcnt} \sum_{k \in K^{CONT}} M_{2,k}$$

Flocculent cost:

$$C_{pur_k} = \pi_{Flcnt} M_{5,Flcnt}$$

Volume of flocculation unit:

$$Q_{c_{flc}} = \theta_{flc}^R \left[\sum_{k \in K^S} \left(\frac{M_{2,k}}{\rho_k} \right) \right]$$

Power required in flocculation unit:

$$PW_{flc} = W_{sp_{flc}} Q_{c_{flc}}$$

Primary Stage Model Equations for Technologies

Sedimentation (sdm):

Efficiency equation:

$$\eta_{sdm} = \frac{M_{13,k}}{M_{9,k}} ; k \in K^{CONT}$$

Concentration factor (CF_{sdm}):

$$CF_{sdm} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in K^{SP}} \left(\frac{M_{13,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{sdm} \left[\sum_{k \in K^{SP}} \left(\frac{M_{13,k}}{\rho_k} \right) \right] = \left[\sum_{k \in K^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]$$

$$2 \leq CF_{sdm} \leq 15$$

$$\text{Written as: } CF_{sdm} \leq 15y_{sdm} \text{ and } CF_{sdm} \geq 2y_{sdm}$$

Area of sedimentation unit:

$$Q_{c_{sdm}} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]}{SOR_{sdm}}$$

Power required in sedimentation unit:

$$PW_{sdm} = W_{sp_{sdm}} Q_{c_{sdm}}$$

Filtration (ftt):

Retention factor equation

$$\xi_{ftt_k} = \frac{M_{11,k}}{M_{8,k}} ; k \in \mathbf{K}^{SP}$$

$$\text{Written as: } \xi_{ftt_k} M_{8,k} = M_{11,k}$$

Concentration factor equation (ftt):

$$CF_{ftt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{8,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{11,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{ftt} \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{13,k}}{\rho_k} \right) \right] = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]$$

$$1 \leq CF_{ftt} \leq 30$$

$$\text{Written as: } CF_{ftt} \leq 30y_{ftt} \text{ and } CF_{ftt} \geq 1y_{ftt}$$

Area of filtration unit (flux balance):

$$Qc_{ftt} = A_{ftt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{8,k}}{\rho_k} \right) \right] (CF_{ftt} - 1)}{\xi_{ftt} CF_{ftt}}$$

$$\text{Written as: } Qc_{ftt} \xi_{ftt} CF_{ftt} = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{8,k}}{\rho_k} \right) \right] (CF_{ftt} - 1)$$

Power requirements for filtration unit:

$$PW_{ftt} = W_{sp_{ftt}} Qc_{ftt}$$

Secondary Stage Model Equations for Technologies

Membrane Bioreactor:

Retention factor equation

$$\xi_{mbrt_k} = \frac{M_{32,k}}{M_{21,k}} ; k \in \mathbf{K}^{SP}$$

$$\text{Written as: } \xi_{mbrt_k} M_{8,k} = M_{11,k}$$

Concentration factor equation (fft):

$$CF_{mbrt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{32,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{mbrt} \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{32,k}}{\rho_k} \right) \right] = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right]$$

$$1.01 \leq CF_{mbrt} \leq 35$$

$$\text{Written as: } CF_{mbrt} \leq 35 y_{mbrt} \text{ and } CF_{mbrt} \geq 1.01 y_{mbrt}$$

Volume of membrane bioreactor:

$$V_{mbrt} = \theta_{mbrt}^R \left[\sum_{k \in \mathbf{K}^S} \left(\frac{M_{21,k}}{\rho_k} \right) \right]$$

Area for membrane for membrane bioreactor unit:

$$Qc_{mbrt} = A_{mbrt} = \left(\frac{V_{mbrt}}{D_{mbrt}} \right)$$

$$\text{Written as: } A_{mbrt} D_{mbrt} = V_{mbrt}$$

Flux balance for membrane bioreactor unit:

$$\zeta_{mbrt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right] (CF_{mbrt} - 1)}{A_{mbrt} CF_{mbrt}}$$

$$\text{Written as: } A_{mbrt} \zeta_{mbrt} CF_{mbrt} = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right] (CF_{mbrt} - 1)$$

Power requirements for membrane bioreactor unit:

$$PW_{mbrt} = WSP_{mbrt} Qc_{mbrt}$$

Adsorption:

Efficiency equation:

$$\eta_{ads} = \frac{M_{23,k}}{M_{17,k}} ; k \in \mathbf{K}^{CONT}$$

Volume of adsorption unit:

$$Qc_{ads} = V_{ads} = \theta_{ads}^R \left[\sum_{k \in \mathbf{K}^S} \left(\frac{M_{17,k}}{\rho_k} \right) \right]$$

Mass of granulated activated carbon (gac) required for adsorption unit:

$$M_{gac,ads} = \rho_{gac} Qc_{ads}$$

Power required for adsorption unit:

$$PW_{ads} = W_{sp_{ads}} Qc_{ads}$$

Activated Sludge:

Efficiency equation:

$$\eta_{asl} = \frac{M_{25,k}}{M_{18,k}} ; k \in \mathbf{K}^{CONT}$$

Volume of activated sludge unit:

$$Qc_{asl} = V_{asl} = \theta_{asl}^R \left[\sum_{k \in \mathbf{K}^S} \left(\frac{M_{18,k}}{\rho_k} \right) \right]$$

Biomass production in activated sludge unit:

$$X_{asl} = \left(\frac{Srt_{asl} \gamma_{asl} \sum_{k \in \mathbf{K}^{CONT}} (M_{18,k} - M_{26,k})}{\theta_{asl}^R [1 + \kappa d_{asl} Srt_{asl}] \sum_{k \in \mathbf{K}^S} \left(\frac{M_{18,k}}{\rho_k} \right)} \right)$$

$$\text{Written as: } X_{asl} \theta_{asl}^R [1 + \kappa d_{asl} Srt_{asl}] \sum_{k \in \mathbf{K}^S} \left(\frac{M_{18,k}}{\rho_k} \right) = Srt_{asl} \gamma_{asl} \sum_{k \in \mathbf{K}^{CONT}} (M_{18,k} - M_{26,k})$$

Solid retention time in activated sludge unit:

$$Srt_{asl} = \left(\frac{V_{asl} X_{asl}}{M_{25, Ssl ds}} \right)$$

Power required for activated sludge unit:

$$PW_{asl} = W_{sp_{asl}} Qc_{asl}$$

Rotating Biological Contactors:

Efficiency equation:

$$\eta_{rbc} = \frac{M_{27,k}}{M_{19,k}} ; k \in K^{CONT}$$

Area of Rotating Biological Contactor unit:

$$Q_{c_{rbc}} = A_{rbc} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{19,k}}{\rho_k} \right) \right]}{\chi_{rbc}}$$

Power required for Rotating Biological Contactor unit:

$$PW_{rbc} = W_{sp_{rbc}} Q_{c_{rbc}}$$

Disinfection:

Efficiency equation:

$$\eta_{dis} = \frac{M_{29,k}}{M_{20,k}} ; k \in K^{CONT}$$

Mass of disinfectant required for disinfection unit

$$M_{31,L_Chltn} = \Phi_{L_Chltn} \sum_{k \in K^{CONT}} M_{20,k}$$

Volume of disinfection unit:

$$Q_{c_{dis}} = V_{dis} = \theta_{dis}^R \left[\sum_{k \in K^S} \left(\frac{M_{20,k}}{\rho_k} \right) \right]$$

Power required for disinfection unit:

$$PW_{dis} = W_{sp_{dis}} Q_{c_{dis}}$$

Tertiary Stage Model Equations for Technologies

Advanced Oxidation Processes:

Mass of ozone needed for advanced oxidation processes unit

$$M_{42,Oz} = \Phi_{Oz} \sum_{k \in K^{CONT}} M_{31,k}$$

Efficiency equation:

$$\eta_{aop} = \frac{M_{40,k}}{M_{36,k}}; k \in K^{CONT}$$

Volume of advanced oxidation processes unit:

$$Q_{c_{aop}} = V_{aop} = \theta_{aop}^R \left[\sum_{k \in K^S} \left(\frac{M_{36,k}}{\rho_k} \right) \right]$$

Power required for advanced oxidation processes unit:

$$PW_{aop} = W_{sp_{aop}} Q_{c_{aop}}$$

Membrane Processes:

Retention factor equation

$$\xi_{mbr_k} = \frac{M_{46,k}}{M_{38,k}}; k \in K^{SP}$$

$$\text{Written as: } \xi_{mbr_k} M_{38,k} = M_{46,k}$$

Concentration factor equation (mbr):

$$CF_{mbr} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in K^{SP}} \left(\frac{M_{46,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{mbr} \left[\sum_{k \in K^{SP}} \left(\frac{M_{46,k}}{\rho_k} \right) \right] = \left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right]$$

$$1 \leq CF_{mbr} \leq 35$$

$$\text{Written as: } CF_{mbr} \leq 35y_{mbr} \text{ and } CF_{mbr} \geq 1y_{mbr}$$

Area of membrane processes unit (flux balance):

$$Q_{c_{mbr}} = A_{mbr} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right] (CF_{mbr} - 1)}{\xi_{mbr} CF_{mbr}}$$

$$\text{Written as: } Qc_{mbr} \zeta_{mbr} CF_{mbr} = \left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right] (CF_{mbr} - 1)$$

Power requirements for membrane unit:

$$PW_{mbr} = W_{sp_{mbr}} Qc_{mbr}$$

Bleaching:

Efficiency equation:

$$\eta_{blc} = \frac{M_{43,k}}{M_{37,k}} ; k \in K^{CONT}$$

Mass of disinfectant required for disinfection unit

$$M_{45,NaClO} = \Phi_{NaClO} \sum_{k \in K^{CONT}} M_{37,k}$$

Volume of disinfection unit:

$$Qc_{dis} = V_{dis} = \theta_{dis}^R \left[\sum_{k \in K^S} \left(\frac{M_{37,k}}{\rho_k} \right) \right]$$

Power required for disinfection unit:

$$PW_{dis} = W_{sp_{dis}} Qc_{dis}$$

Cost Model Equations

Stagewise Cost Equations

Annualized capital cost in each stage:

$$CCAC_{Nstg} = 1.66 \zeta_{RF} BMC_{mult} \sum_{i \in \text{istg}\{1,2,3,4\}} C_{ei}$$

Material Cost:

$$CCRM_{s1} = [\tau_{ann}(C_{pur_{Flcnt}})]$$

$$CCRM_{s2} = 0$$

$$CCRM_{s3} = [\tau_{ann}(C_{pur_{Lchtrn}})]$$

$$CCRM_{s4} = [\tau_{ann}(C_{pur_{Oz}} + C_{pur_{NaClO}})]$$

Consumable Cost:

$$CCCS_{s1} = 0$$

$$CCCS_{s2} = Cons_{ftt}$$

$$CCCS_{s3} = Cons_{ads} + Cons_{mbrt}$$

$$CCCS_{s4} = Cons_{mbr}$$

Labor Cost

$$CCLC_{Nstg} = \tau_{ann} C_{Lab} \sum_{i \in istg\{1,2,3,4\}} Nlb_i$$

Utility Cost

$$CCUC_{Nstg} = \tau_{ann} C_{elec} \sum_{i \in istg\{1,2,3,4\}} PW_i$$

Other Cost

$$CCOC_{Nstg} = 2.78 \tau_{ann} C_{Lab} \sum_{i \in istg\{1,2,3,4\}} Nlb_i$$

Total Cost in each Stage

$$CCTC_{Nstg} = CCAC_{Nstg} + CCRM_{Nstg} + CCCS_{Nstg} + CCLC_{Nstg} + CCUC_{Nstg} + CCOC_{Nstg}$$

Total Category Cost:

$$CCTAC = \sum_{n \in Nstg\{1,2,3,4\}} CCAC_n$$

$$CCTRM = \sum_{n \in Nstg\{1,2,3,4\}} CCRM_n$$

$$CCTCS = \sum_{n \in Nstg\{1,2,3,4\}} CCCS_n$$

$$CCTLc = \sum_{n \in Nstg\{1,2,3,4\}} CCLC_n$$

$$CCTUC = \sum_{n \in Nstg\{1,2,3,4\}} CCUC_n$$

$$CCTOC = \sum_{n \in Nstg\{1,2,3,4\}} CCOC_n$$

$$CCTPC = CCTAC + CCRM + CCTCS + CCTLc + CCTUC + CCTOC$$

Objective Function 1:

$$Obj = \text{Min } CCTPC$$

A.2 Model parameters and input data

Table A.2.1 Density and Molecular Weight of Components

Component	Value (kg/m ³)	Value (kg/kmol)
Water	1000	18
Solid particles	1800	102
Metals	2500	98
Chemicals	1100	48
Ozone	2.14	48
Sodium Hypochlorite	1110	74.44
Flocculant	2200	2200
Liquid chlorine	1470	70.91

Table A.2.2 Purchase cost of added components

Component	Value (\$/kg)
Ozone	3.53
Sodium Hypochlorite	0.35
Flocculant	0.75
Liquid chlorine	2

Table A.2.3 Standard capacity, cost, laborers, and power for technologies

Unit Operation (costing capacity)	Standard Capacity (Units)	Standard Capacity Cost (million \$)	Standard Laborers Required (#/h)	Standard Power Required (kW/h)
Flocculation (Volume)	2000 (m ³)	0.538	0.1	0.0002
Filtration (Area)	80 (m ²)	0.039	0.5	0.1
Sedimentation (Volume)	2500 (m ³)	1.128	0.1	0.0002
Adsorption (Volume)	100 (m ³)	0.12	0.2	0.3
Membrane Bioreactor (Area)	40 (m ²)	1.194	0.1	0.2
Rotational Biological Container (Area)	185 (m ²)	0.045	0.3	0.01
Activated Sludge (Volume)	250 (m ³)	0.569	0.4	0.2
Disinfection (Volume)	540 (m ³)	0.627	0.7	0.5
Membrane Processes (Area)	80 (m ²)	0.938	0.5	0.2
Advanced Oxidation Processes (Volume)	1000 (m ³)	0.735	0.1	0.5
Bleaching (Volume)	500 (m ³)	0.100	0.5	0.33

Table A.2.4 Replacement time for technologies with consumables

Technology	Value (h/yr)
Filtration	2000
Adsorption	720
Membrane Processes	1000
Membrane Bioreactor	1000

Table A.2.5 Replacement cost for technologies with consumables

Technology	Value (\$/Unit)
Filtration	100
Adsorption	74.16
Membrane Processes	400
Membrane Bioreactor	400

A.2.6 Flocculation (flc):

Flocculent added (kg/kg) – 0.005

Residence time (h) – 0.5

A.2.7 Sedimentation (sdm):

Efficiency – 80%

Depth – 3m

A.2.8 Filtration (ftt):

Retention factor: Water – 0.05, Solids – 0.80, Metals – 0.10, Chemicals – 0.05

Flux (m³/m².h): 0.2

A.2.9 Membrane Bioreactor (mbrt):

Retention factor: Water – 0.005, Solids – 0.95, Metals – 0.85, Chemicals – 0.50

Flux (m³/m².h): 0.025

A.2.10 Adsorption (ads):

Empty bed contact time (h): 0.25

Density of granular activated carbon (GAC) (kg/m³): 1030

Efficiency: 90%

Void fraction of GAC: 50%

A.2.11 Activated Sludge (asl):

Decay of biomass coefficient (h⁻¹): 0.0021

Biomass yield (kg/kg): 0.5

Hydraulic retention time (h): 2

Efficiency: 80%

A.2.12 Rotating Biological Contactors (rbc):

Efficiency: 80%

Hydraulic loading (m³/m².h): 20

A.2.13 Disinfection (dis):

Efficiency: 95%

Ratio of liquid chlorine to contaminant (kg/kg): 0.00173

Residence time (h): 2

A.2.14 Advanced Oxidation Processes (aop):

Ratio of ozone to contaminant (kg/kg): 0.000173

Efficiency: 98%

Residence time (h): 0.21

A.2.15 Membrane Processes (mbr):

Retention factor: Water – 0.05, Solids – 0.90, Metals – 0.90, Chemicals – 0.95

Flux (m³/m².h): 0.0856**A.2.16 Bleaching (blc):**

Efficiency: 98%

Ratio of sodium hypochlorite to contaminant (kg/kg): 0.00173

Residence time (h): 2

A.3 Integer-cuts for determining 1st, 2nd, and 3rd best configuration

$$\sum_{y_{ibv}=1} y_{ibv} - \sum_{y_{ibv}=0} y_{ibv} \leq (\# \text{ of } 1' \text{ in solution}) - 1$$

First integer-cut to determine first best alternative:

$$[y_{blc} + y_{sdm} + y_{flc} + y_{ads}] - [y_{ftt} + y_{asl} + y_{rbc} + y_{mbrt} + y_{aop} + y_{mbr} + y_{dis}] \leq 4 - 1$$

Second integer-cut to determine the second best alternative

$$[y_{blc} + y_{sdm} + y_{flc} + y_{dis}] - [y_{ftt} + y_{asl} + y_{rbc} + y_{mbrt} + y_{aop} + y_{mbr} + y_{ads}] \leq 4 - 1$$

Third integer-cut to determine third-best alternative:

$$[y_{blc} + y_{ftt} + y_{flc} + y_{dis}] - [y_{sdm} + y_{asl} + y_{rbc} + y_{mbrt} + y_{aop} + y_{mbr} + y_{ads}] \leq 4 - 1$$

A.4 Cost Distribution**Table A.3.1 Breakdown of Stage-wise Cost of Purification**

Cost Category	Stage-wise Cost Distribution			
	Pretreatment	Primary	Secondary	Tertiary
Annualized Capital Cost(\$/y)	4.81E+04	6.42E+04	4.59E+04	5.16E+04
Material Cost(\$/y)	5.97E+05	0.00E+00	0.00E+00	4.58E+05
Consumable Cost(\$/y)	0.00E+00	0.00E+00	1.98E+04	0.00E+00
Labor Cost (\$/y)	6.61E+02	3.37E+02	1.16E+04	4.53E+04
Utilities Cost(\$/y)	8.81E+00	5.61E+00	5.78E+03	4.98E+04
Other Cost(\$/y)	1.18E+03	2.04E+04	2.06E+04	8.05E+04
Total(\$/y)	6.47E+05	8.50E+04	1.04E+05	6.85E+05
Percentage Distribution				
Annualized capital cost	7.43%	75.56%	44.28%	7.54%
Raw material cost	92.28%	0.00%	0.00%	66.82%
Consumable cost	0.00%	0.00%	19.14%	0.00%
Labor cost	0.10%	0.40%	11.15%	6.61%
Utilities Cost	0.00%	0.01%	5.58%	7.27%
Other Cost	0.18%	24.04%	19.85%	11.76%
Total	100.00%	100.00%	100.00%	100.00%

A.5 Sustainable Process Index (SPI) Calculations

A.5.1 SPI for Municipal Wastewater Treatment

Parameters

F_{RR} (kg/yr)	- feed of a processed resource (752400000)
y_R (kg/m ² .yr)	- specific yield (243.1542)
$y_{EI,RN}$ (kWh/m ² .yr)	- mean industrial energy yield or mean industrial energy supply density (7)
F_{RN} (kg/yr)	- feed of a processed resource (2172028)
C_N (\$/kg)	- price of the material (world market price, taxes excluded) (7)
C_E (\$/kWh)	- price of one kilowatt-hour of energy (industrial price, taxes excluded) (0.1)
F_E (kWh/yr)	- energy used in the process (555659.28)
y_E (kWh/m ² .yr)	- energy yield (43)
C_I (\$)	- total cost of energy for indirect installation (122720)
LS (yr)	- depreciated area over the life-span years (30)
$y_{EI,II}$ (kWh/m ² .yr)	- industrial energy supply density or yield (43)
N_S (cap/yr)	- total number of workers in the treatment plant (80.19)
y_S (cap/m ² .yr)	- yield factor due to staff (3.59E-05)
$c_{c,m}$ (kg _m /kg)	- allowable concentration of substance, m [Solids, Chemical, Metals, Water] in the compartment, c [air, water, soil]
R_c (kg/m ² .yr)	- rate of renewal of the environmental compartments, c [air, water, soil]

Estimated Parameters

$E_{D,RN}$ - energy demand to supply one kilogram of the material in question for non-renewable energy (kWh/kg)

$$E_{D,RN} = \frac{0.95 C_N}{C_E} = \frac{0.95 \times 7}{0.1} = 66.5$$

$E_{D,II}$ - energy demand to supply one kilogram of the material in question for indirect land energy (kWh/yr)

$$E_{D,II} = \frac{0.54 C_I}{C_E \cdot LS} = \frac{0.54 \times 122720}{0.1 \times 30} = 22089.6$$

$S_{c,m}$ - dissipation to potential sink (kg_m/m².yr)

$$S_{c,m} = R_c \cdot c_{c,m}$$

Analysis for R_{soil} (kg/m².yr)

Rate of soil renewal (RSN) in the US is 2.2E-04 m/yr

Assuming the soil is loamy with a 50% pore space, then the bulk density is 1330 kg/m³

$$R_{soil} = RSN \times Den_{bulk} = 0.00022 \times 1330 = 0.2926$$

Since we categorized contaminants into of solids, chemicals, and metals, we used contaminants that had the smallest allowable concentration for each category in the compartments to estimate S. For solids contaminant, we used lead (Pb), for chemical we used Chromium (Cr), and for metals we used lead (Pb).

Analysis for $S_{soil,m}$ (kgm/m².yr)

$$S_{soil,m} = R_{soil} \cdot C_{soil,m}$$

Component (m)	C _(soil,m) (kgm/kg)	S _(soil,m) (kgm/m ² .y)
Solids (Sslds)	1.00E+00	2.93E-01
Chemical (Chem)	1.00E-04	2.93E-05
Metals (Mtls)	2.00E-06	5.85E-07
Water (Wtr)	1.00E+00	2.93E-01

Analysis for R_{water} (kg/m².yr)

Average rate of precipitation (RP) form Jan, 2009 to Dec, 2019 in the US is 31.91 in/yr (0.810514 m/yr)

Seeping ratio (SR) of water is 0.30

$$R_{water} = RP \times SR \times Den_{water} = 0.810514 \times 0.30 \times 1000 = 243.1542$$

Analysis for $S_{water,m}$ (kgm/m².yr)

$$S_{water,m} = R_{water} \cdot C_{water,m}$$

Component (m)	C _(water,m) (kgm/kg)	S _(water,m) (kgm/m ² .y)
Solids (Sslds)	1.67E-06	4.05E-04
Chemical (Chem)	1.00E-07	2.43E-05
Metals (Mtls)	1.50E-08	3.65E-06
Water (Wtr)	1.00E+00	2.43E+02

$$S_{air,chem} \text{ (kgm/m}^2\text{.yr)} = 6.50E-03$$

$FP_{c,m}$ product flow rate to compartment c, by substance, m (kg_m/yr) [from GAMS code]

Component (m)	Fraction of m into compartment c			$FP_{c,m}$		
	Air	Water	Soil	Air	Water	Soil
Solids (Sslds)	0	0.05	0.95	0.00E+00	3.17E+03	6.02E+04
Chemical (Chem)	0.03	0.9	0.07	9.50E+00	2.85E+02	2.22E+01
Metals (Mtls)	0	0.7	0.3	0.00E+00	2.22E+01	9.50E+00
Water (Wtr)	0	0.95	0.05	0.00E+00	7.15E+08	3.76E+07

Variables

A_R - area for raw material production (m²/yr)

A_{RR} - area for renewable raw material production (m²/yr)

A_E - area for energy production (m²/yr)

A_I - area for installation for equipment and other infrastructure (m²/yr)

A_{ID} - area for direct installation (m²/yr)

A_{II} - area for indirect installation (m²/yr)

A_S - area for staff (m²/yr)

$A_{P,c,m}$ - area for dissipating a single component of particular product flow to a given compartment (m²/yr)

$A_{PS,c}$ - area assigned to the dissipation of a particular product stream, S (m²/yr)

A_P - area for product dissipation (m²/yr)

A_{tot} - total area (m²/m³WW-yr)

Area for Raw Material Production (A_R)

Area for Renewable Raw Material Production (A_{RR})

$$A_{RR} = \frac{F_{RR}}{Y_R} = \frac{7524000000}{243.1542} = 3.09E06$$

Area for Non-Renewable Raw Material Production (A_{RN})

$$A_{RN} = \frac{F_{RN} \cdot E_{D,RN}}{Y_{EI,RN}} = \frac{2172028 \times 66.5}{7} = 2.06E07$$

$$A_R = A_{RR} + A_{RN} = 2.37E07$$

Area for Energy Production (A_E)

$$A_E = \frac{F_E}{Y_E} = \frac{555659.28}{43} = 1.29E4$$

Area for Installations (A_I)

$$A_I = A_{ID} + A_{II}$$

Area for Direct Installation (A_{ID})[from GAMS Code]

Flocculation technology = 18.54

Sedimentation technology = 35.43

Adsorption technology = 4.86

Bleaching technology = 38.09

$$A_{ID} = 96.91$$

Area for Indirect Installation (A_{II})

$$A_{II} = \frac{E_{D,II}}{Y_{EI,II}} = \frac{22089.6}{43} = 5.14E2$$

Area for Staff (A_S)

$$A_S = N_S \cdot a_{in} = \frac{N_S}{Y_S} = \frac{80.19}{0.0000359} = 2.23E6$$

Area for Product Dissipation into Various Environmental Compartment (A_P)

$$A_{P,c,m} = \frac{F_{P,c,m}}{S_{c,m}}$$

Component (m)	$A_{P,c,m}$		
	Air	Water	Soil
Solids (Sslds)	--	7.82E+06	2.06E+05
Chemical (Chem)	1.46E+03	1.17E+07	7.58E+05
Metals (Mtls)	--	6.08E+06	1.62E+07
Water (Wtr)	--	2.94E+06	1.29E+08

$$A_{P,S,c} = \max_m(A_{P,c,m})$$

Highlighted are the maximum values for each component

Component (m)	$A_{P,c,m}$		
	Air	Water	Soil
Solids (Sslds)	--	7.82E+06	2.06E+05
Chemical (Chem)	1.46E+03	1.17E+07	7.58E+05
Metals (Mtls)	--	6.08E+06	1.62E+07
Water (Wtr)	--	2.94E+06	1.29E+08

$$A_P = \sum_c A_{P,S,c} = 1.40E8$$

$$A_{tot} = A_R + A_E + A_I + A_S + A_P = 2.10E+02 \text{ (m}^2\text{/m}^3\text{WW-yr)}$$

A.5.2 SPI for Direct Disposal of Municipal Wastewater

We considered on the area needed to sustainably embed the wastewater into the ecosystem, i.e. A_P

Area for Product Dissipation into Various Environmental Compartment (A_P)

$F_{P,c,m}$ product flow rate to compartment c, by substance, m (kg_m/yr) [from GAMS code]

Component (m)	Fraction of		$F_{P,c,m}$	
	Water	Soil	Water	Soil
Solids (Sslds)	0.05	0.95	8.76E+06	1.66E+08
Chemical (Chem)	0.95	0.05	8.32E+05	4.38E+04
Metals (Mtls)	0.7	0.3	6.13E+04	2.63E+04
Water (Wtr)	0.95	0.05	8.32E+08	4.38E+07

$$A_{P,c,m} = \frac{F_{P,c,m}}{S_{c,m}}$$

Component (m)	$A_{P,c,m}$	
	Water	Soil
Solids (Sslds)	7.82E+06	2.06E+05
Chemical (Chem)	1.17E+07	7.58E+05
Metals (Mtls)	6.08E+06	1.62E+07
Water (Wtr)	2.94E+06	1.29E+08

$$A_{P,S,c} = \max_m(A_{P,c,m})$$

Highlighted are the maximum values for each component

Component (m)	A _{P,c,m}	
	Water	Soil
Solids (Sslds)	2.16E+10	5.69E+08
Chemical (Chem)	3.42E+10	1.50E+09
Metals (Mtls)	1.68E+10	4.49E+10
Water (Wtr)	3.42E+06	1.50E+08

$$A_P = \sum_c A_{P,S,c} = 7.91E10$$

$$A_{tot} = A_P = 9.03E+04 \text{ (m}^2\text{/m}^3\text{WW-yr)}$$

B. Information for Pharmaceutical Case Study

B.1 Model equations and details

- a) The uppercase italic Latin fonts (not colored) are for variables (optimization variables)
- b) The uppercase Latin font and lowercase Greek fonts in red are the specified input parameters
- c) Parameters evaluated from available inputs are the uppercase Latin fonts and lowercase Greek fonts in color green.
- d) The parameter or variable to be evaluated is always on the L.H.S of the equation

B.1.1 Indices and Sets

$i \in I$ – technologies (used as subscript to variables)

<i>flc</i>	-	flocculation,
<i>sdm</i>	-	sedimentation,
<i>ftt</i>	-	filtration,
<i>ads</i>	-	adsorption,
<i>asl</i>	-	activated sludge,
<i>rbc</i>	-	rotating biological contactors,
<i>dis</i>	-	disinfection,
<i>mbrt</i>	-	membrane bioreactor,
<i>aop</i>	-	advanced oxidation process,
<i>blc</i>	-	bleaching,
<i>mbr</i>	-	membrane processes
<i>splt#</i>	-	splitter and # = {1, 2, 3, 4}
<i>mrx#</i>	-	mixer and # = {1, 2, 3, 4}
<i>byp#</i>	-	bypass and # = {1, 2, 3, 4}}

$j \in J$ – stream (used as subscript to variables)

{1, 2, 3, 4,, 49}

$k \in K$ – components (used as subscript to variables)

<i>Wtr</i>	-	water,
<i>Ssld</i>	-	solids,
<i>Mtls</i>	-	metals
<i>Chem</i>	-	chemicals
<i>API</i>	-	active pharmaceutical ingredients
<i>Flcnt</i>	-	flocculants,
<i>Oz</i>	-	ozone,
<i>NaClO</i>	-	sodium hypochlorite,
<i>L_Chln</i>	-	liquid chlorine}

$s \in S$ - stages {s1, s2, s3, s4}

B.1.2 Subsets

Subsets for technologies

- I^{CST} – technologies with costs
{*flc, sdm, ftt, ads, asl, rbc, mbrt, dis, mbr, blc* }
- I^{CF} – technologies with concentration factor
{*ftt, mbrt, sdm, mbr*}
- I^{CONS} – technologies with consumables
{*ftt, ads, mbrt, mbr*}
- I^{EAC} – technologies with externally added components
{*flc, aop, dis, blc*}
- I^{BV} – technologies with binary variables
{*flc, sdm, ftt, ads, asl, rbc, mbrt, dis, mbr, blc, byp1, byp2, byp3, byp4* }
- I^{S1} – technologies in stage 1
{*flc, byp1*}
- I^{S2} – technologies in stage 2
{*ftt, sdm, byp2*}
- I^{S3} – technologies in stage 3
{*ads, asl, rbc, dis, mbrt, byp3*}
- I^{S4} – technologies in stage 4
{*aop, blc, mbr, byp4*}

Subsets for streams

- J^{flc} – streams for flocculation
{2, 4, 5}
- J^{byp1} – streams for bypass 1
{3, 6}
- J^{sdm} – streams for sedimentation
{9, 13, 14}
- J^{ftt} – streams for filtration
{8, 11, 12}
- J^{byp2} – streams for bypass 2
{10, 15}
- J^{ads} – streams for adsorption
{17, 23, 24}

- J^{asl} – streams for activated sludge
{18, 25, 26}
- J^{rbc} – streams for rotating biological containers
{19, 27, 28}
- J^{dis} – streams for disinfection
{20, 29, 30, 31}
- J^{mbrt} – streams for membrane bioreactor
{21, 32, 33}
- J^{byp3} – streams for bypass 3
{22, 34}
- J^{aop} – streams for advanced oxidation process
{36, 40, 41, 42}
- J^{mbr} – streams for membrane processes
{38, 46, 47}
- J^{blc} – streams for bleaching
{37, 43, 44, 45}
- J^{byp4} – streams for bypass 4
{39, 48}

Subsets for components

- K^S – components in streams
{*Wtr, Ssld, Mtls, Chem, API, Flcnt, Oz, NaClO, L_Chln*}
- K^{SP} – components in initial wastewater stream
{*Wtr, Ssld, Mtls, Chem, API*}
- K^{CONT} – components that are contaminants
{*Ssld, Mtls, Chem, API*}
- K^{EAC} – components that are externally added
{*Flcnt, Oz, NaClO, L_Chln*}

B.1.3 Dynamic sets for connectivity

- J_i - streams of technology i
- J_{in_i} - inlet streams of technology i
- J_{out_i} - outlet streams of technology i
- K_i - components k in technology i
- K_j - components k in stream j

B.1.4 Model Parameters

General Parameters

ρ_k (kg/m³) = Density of component k

π_{WW} (m³ WW/h) = Entering volumetric flowrate of wastewater (WW)

π^{Rep}_i (\$/unit) = Replacement cost of consumables per unit capacity in technology i

μ (N-s/m²) = viscosity of fluid

η_i (%) = efficiency of technology i

θ_i^R (hr) – residence time in technology i

θ_i^{Rep} (h/year) = Replacement time for consumables in technology i

τ_{ann} (h/annum) = annual operation in hours (330 day x 24 h/day = 7920 hrs)

$C0_i$ (\$/capacity) = standard capacity cost in technology i

g (m/s²) = gravitational constant

nc = cost scaling index (2/3 rule)

$Nlabr_i$ (#/h) = standard # of laborers required for technology i per hour

$Q0_i$ (m³ or m² or m³/h) = standard capacity of technology i

MW_k (kg/kmol) = molecular weight of component k

Min_k (kg/m³) = initial mass concentration of component k

$Cpur_k$ (\$/kg) = purchase cost of added component k

Wsp_i (kW/h) = standard power required for technology i per hour

MM_k (--) = Big-M constant for component k

Φ_k (kg/kg WW) = amount of externally added component k

dp (m) = diameter of particle

$\xi_{j,i}$ (--) = retention factor of component k for technology i {*ftt*, *mbrt*, and *mbr* technologies}

ζ_{RF} (--) = capital recovery/ charge factor (0.11)

ζ_i (m³/m²h) = flux of technology i {*ftt*, *mbrt*, and *mbr* technologies}

κd_i (h⁻¹) = decay of biomass coefficient of technology i {*asl* technology}

γ_i (kg/kg) = biomass yield of technology i {*asl* technology}

χ_i (m³/m²h) = hydraulic loading of technology i {*rbc* technology}

BMC_{mult} (--) = bare module cost multiplier (5.4)

C_{Lab} (\$/h) = labor cost – operator basis (30)

C_{Elec} (\$/kW) = cost of electricity per hour (0.1)

Evaluated Parameters

SOR_i (m/s) = surface overflow rate id sedimentation

U_i (m/s) = settling velocity of technology i

B.1.5 Model Variables

General Variables

Cc_i (\$) = Purchase cost of technology $i \in I^{CST}$

CF_i (m³/m³) = Concentration factor for technologies $i \in I^{CF}$

Cpr_k (\$/h) = Purchase cost of added components $k \in K^{EAC}$

$M_{j,k}$ (kg/h) = Mass flowrate of component k in stream j

Qc_i (m³ or m² or m³/h) = capacity cost of technologies $i \in I^{CST}$

PW_i (kW/h) = power requirements for technologies $i \in I^{CST}$

$Nlbr_i$ (#/h) = number of laborers required for technology $i \in I^{CST}$

Yo_i (kg/kg) = observed bacteria yield of technology i (*asl* technology)

Sr_i (m/h) = settling rate of unit i (*asl* technology)

X_i (kg/h) = biomass produced in technology i (*asl* technology)

Srt_i (h) = solids residence time in technology i (*asl* technology)

D_i (m) = diameter of technology i (*mbrt* technology)

$Cons_i$ (\$/annum) = consumable cost of technology $i \in I^{CONS}$

Binary Variables

y_i (--) = binary variables for technologies to selected $i \in I^{BV}$

Stage-wise Costing Variables

$CCAC_{Nstg}$ = annualized capital (fixed) cost in nth stage

$CCRM_{Nstg}$ = material cost in nth stage

$CCCS_{Nstg}$ = consumable cost in nth stage

$CCLB_{Nstg}$ = labor cost in nth stage

$CCUT_{Nstg}$ = utility cost in nth stage

$CCOT_{Nstg}$ = other cost in nth stage (plant overhead and supervision costs)

$CCTC_{Nstg}$ = total cost in nth stage (all cost added in that particular stage)

$CCTPC$ = total cost for process (summation of total cost in each stage)

B.1.6 Model Equations:

Initial wastewater flowrate equations:

$$M_{1,k} = (\sum_k Min_k) \pi_{WW}; \forall k \in K^{SP}$$

Component balances in all technologies:

$$\sum_{j \in J_{in_i}} M_{j,k} = \sum_{j \in J_{out_i}} M_{j,k}; \forall k \in K^S$$

Cost of technologies:

$$\left(\frac{C_{c_i}}{CO_i} \right) = \left(\frac{Q_{c_i}}{QO_i} \right)^{nc}; \forall i \in I^{CST}$$

Labor requirements in technologies:

$$Nlbr_i QO_i = Nlabr_i Qc_i; \forall i \in I^{CST}$$

Consumable costs in technologies:

$$Cons_i = \frac{\tau_{ann}}{\theta_i^{Rep}} \pi_i^{Rep} Qc_i; \forall i \in I^{CST}$$

Logical equations:

$$M_{i,j} - M1_k y_i \leq 0; \forall i \in I^{BV}, j \in J, k \in K_i \text{ and } K_j$$

Selection of technologies in each stage:

Preliminary (Pretreatment) stage:

$$y_{flc} + y_{byp,1} = 1$$

Primary Treatment Stage:

$$y_{ftt} + y_{sdm} + y_{byp,2} = 1$$

Secondary Treatment Stage:

$$y_{ads} + y_{asl} + y_{rbc} + y_{dis} + y_{mbrt} + y_{byp,3} = 1$$

Tertiary Treatment Stage:

$$y_{aop} + y_{mbr} + y_{blc} = 1$$

Preliminary (Pretreatment) Stage Model Equations for Technologies

Flocculation (flc):

Flocculent added:

$$M_{5,Flcnt} = \Phi_{Flcnt} \sum_{k \in K^{CONT}} M_{2,k}$$

Flocculent cost:

$$C_{pur_k} = \pi_{Flcnt} M_{5,Flcnt}$$

Volume of flocculation unit:

$$Q_{c_{flc}} = \theta_{flc}^R \left[\sum_{k \in K^S} \left(\frac{M_{2,k}}{\rho_k} \right) \right]$$

Power required in flocculation unit:

$$PW_{flc} = W_{sp_{flc}} Q_{c_{flc}}$$

Primary Stage Model Equations for Technologies

Sedimentation (sdm):

Efficiency equation:

$$\eta_{sdm} = \frac{M_{13,k}}{M_{9,k}} ; k \in K^{CONT}$$

Concentration factor (CF_{sdm}):

$$CF_{sdm} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in K^{SP}} \left(\frac{M_{13,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{sdm} \left[\sum_{k \in K^{SP}} \left(\frac{M_{13,k}}{\rho_k} \right) \right] = \left[\sum_{k \in K^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]$$

$$2 \leq CF_{sdm} \leq 15$$

$$\text{Written as: } CF_{sdm} \leq 15y_{sdm} \text{ and } CF_{sdm} \geq 2y_{sdm}$$

Area of sedimentation unit:

$$Q_{c_{sdm}} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]}{SOR_{sdm}}$$

Power required in sedimentation unit:

$$PW_{sdm} = W_{sp_{sdm}} Q_{c_{sdm}}$$

Filtration (ftt):

Retention factor equation

$$\xi_{ftt_k} = \frac{M_{11,k}}{M_{8,k}} ; k \in \mathbf{K}^{SP}$$

$$\text{Written as: } \xi_{ftt_k} M_{8,k} = M_{11,k}$$

Concentration factor equation (ftt):

$$CF_{ftt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{8,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{11,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{ftt} \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{13,k}}{\rho_k} \right) \right] = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{9,k}}{\rho_k} \right) \right]$$

$$1 \leq CF_{ftt} \leq 30$$

$$\text{Written as: } CF_{ftt} \leq 30y_{ftt} \text{ and } CF_{ftt} \geq 1y_{ftt}$$

Area of filtration unit (flux balance):

$$Qc_{ftt} = A_{ftt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{8,k}}{\rho_k} \right) \right] (CF_{ftt} - 1)}{\xi_{ftt} CF_{ftt}}$$

$$\text{Written as: } Qc_{ftt} \xi_{ftt} CF_{ftt} = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{8,k}}{\rho_k} \right) \right] (CF_{ftt} - 1)$$

Power requirements for filtration unit:

$$PW_{ftt} = W_{sp_{ftt}} Qc_{ftt}$$

Secondary Stage Model Equations for Technologies

Membrane Bioreactor:

Retention factor equation

$$\xi_{mbrt_k} = \frac{M_{32,k}}{M_{21,k}} ; k \in \mathbf{K}^{SP}$$

$$\text{Written as: } \xi_{mbrt_k} M_{8,k} = M_{11,k}$$

Concentration factor equation (ftt):

$$CF_{mbrt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{32,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{mbrt} \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{32,k}}{\rho_k} \right) \right] = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right]$$

$$1.01 \leq CF_{mbrt} \leq 35$$

$$\text{Written as: } CF_{mbrt} \leq 35 y_{mbrt} \text{ and } CF_{mbrt} \geq 1.01 y_{mbrt}$$

Volume of membrane bioreactor:

$$V_{mbrt} = \theta_{mbrt}^R \left[\sum_{k \in \mathbf{K}^S} \left(\frac{M_{21,k}}{\rho_k} \right) \right]$$

Area for membrane for membrane bioreactor unit:

$$Qc_{mbrt} = A_{mbrt} = \left(\frac{V_{mbrt}}{D_{mbrt}} \right)$$

$$\text{Written as: } A_{mbrt} D_{mbrt} = V_{mbrt}$$

Flux balance for membrane bioreactor unit:

$$\zeta_{mbrt} = \frac{\left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right] (CF_{mbrt} - 1)}{A_{mbrt} CF_{mbrt}}$$

$$\text{Written as: } A_{mbrt} \zeta_{mbrt} CF_{mbrt} = \left[\sum_{k \in \mathbf{K}^{SP}} \left(\frac{M_{21,k}}{\rho_k} \right) \right] (CF_{mbrt} - 1)$$

Power requirements for membrane bioreactor unit:

$$PW_{mbrt} = WSP_{mbrt} Qc_{mbrt}$$

Adsorption:

Efficiency equation:

$$\eta_{ads} = \frac{M_{23,k}}{M_{17,k}}; k \in K^{CONT}$$

Volume of adsorption unit:

$$Q_{c_{ads}} = V_{ads} = \theta_{ads}^R \left[\sum_{k \in K^S} \left(\frac{M_{17,k}}{\rho_k} \right) \right]$$

Mass of granulated activated carbon (gac) required for adsorption unit:

$$M_{gac,ads} = \rho_{gac} Q_{c_{ads}}$$

Power required for adsorption unit:

$$PW_{ads} = W_{sp_{ads}} Q_{c_{ads}}$$

Activated Sludge:

Efficiency equation:

$$\eta_{asl} = \frac{M_{25,k}}{M_{18,k}}; k \in K^{CONT}$$

Volume of activated sludge unit:

$$Q_{c_{asl}} = V_{asl} = \theta_{asl}^R \left[\sum_{k \in K^S} \left(\frac{M_{18,k}}{\rho_k} \right) \right]$$

Biomass production in activated sludge unit:

$$X_{asl} = \left(\frac{Srt_{asl} Y_{asl} \sum_{k \in K^{CONT}} (M_{18,k} - M_{26,k})}{\theta_{asl}^R [1 + \kappa d_{asl} Srt_{asl}] \sum_{k \in K^S} \left(\frac{M_{18,k}}{\rho_k} \right)} \right)$$

$$\text{Written as: } X_{asl} \theta_{asl}^R [1 + \kappa d_{asl} Srt_{asl}] \sum_{k \in K^S} \left(\frac{M_{18,k}}{\rho_k} \right) = Srt_{asl} Y_{asl} \sum_{k \in K^{CONT}} (M_{18,k} - M_{26,k})$$

Solid retention time in activated sludge unit:

$$Srt_{asl} = \left(\frac{V_{asl} X_{asl}}{M_{25,sslds}} \right)$$

Power required for activated sludge unit:

$$PW_{asl} = W_{sp_{asl}} Q_{c_{asl}}$$

Rotating Biological Contactors:

Efficiency equation:

$$\eta_{rbc} = \frac{M_{27,k}}{M_{19,k}}; k \in K^{CONT}$$

Area of Rotating Biological Contactor unit:

$$Q_{c_{rbc}} = A_{rbc} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{19,k}}{\rho_k} \right) \right]}{\chi_{rbc}}$$

Power required for Rotating Biological Contactor unit:

$$PW_{rbc} = W_{sp_{rbc}} Q_{c_{rbc}}$$

Disinfection:

Efficiency equation:

$$\eta_{dis} = \frac{M_{29,k}}{M_{20,k}} ; k \in K^{CONT}$$

Mass of disinfectant required for disinfection unit

$$M_{31,L_Chlrm} = \Phi_{L_Chlrm} \sum_{k \in K^{CONT}} M_{20,k}$$

Volume of disinfection unit:

$$Q_{c_{dis}} = V_{dis} = \theta_{dis}^R \left[\sum_{k \in K^S} \left(\frac{M_{20,k}}{\rho_k} \right) \right]$$

Power required for disinfection unit:

$$PW_{dis} = W_{sp_{dis}} Q_{c_{dis}}$$

Tertiary Stage Model Equations for Technologies

Advanced Oxidation Processes:

Mass of ozone needed for advanced oxidation processes unit

$$M_{42,Oz} = \Phi_{Oz} \sum_{k \in K^{CONT}} M_{31,k}$$

Efficiency equation:

$$\eta_{aop} = \frac{M_{40,k}}{M_{36,k}} ; k \in K^{CONT}$$

Volume of advanced oxidation processes unit:

$$Q_{c_{aop}} = V_{aop} = \theta_{aop}^R \left[\sum_{k \in K^S} \left(\frac{M_{36,k}}{\rho_k} \right) \right]$$

Power required for advanced oxidation processes unit:

$$PW_{aop} = W_{sp_{aop}} Q_{c_{aop}}$$

Membrane Processes:

Retention factor equation

$$\xi_{mbr_k} = \frac{M_{46,k}}{M_{38,k}}; k \in K^{SP}$$

$$\text{Written as: } \xi_{mbr_k} M_{38,k} = M_{46,k}$$

Concentration factor equation (mbr):

$$CF_{mbr} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right]}{\left[\sum_{k \in K^{SP}} \left(\frac{M_{46,k}}{\rho_k} \right) \right]}$$

$$\text{Written as: } CF_{mbr} \left[\sum_{k \in K^{SP}} \left(\frac{M_{46,k}}{\rho_k} \right) \right] = \left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right]$$

$$1 \leq CF_{mbr} \leq 35$$

$$\text{Written as: } CF_{mbr} \leq 35 y_{mbr} \text{ and } CF_{mbr} \geq 1 y_{mbr}$$

Area of membrane processes unit (flux balance):

$$Q_{c_{mbr}} = A_{mbr} = \frac{\left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right] (CF_{mbr} - 1)}{\xi_{mbr} CF_{mbr}}$$

$$\text{Written as: } Q_{c_{mbr}} \xi_{mbr} CF_{mbr} = \left[\sum_{k \in K^{SP}} \left(\frac{M_{38,k}}{\rho_k} \right) \right] (CF_{mbr} - 1)$$

Power requirements for membrane unit:

$$PW_{mbr} = W_{sp_{mbr}} Q_{c_{mbr}}$$

Bleaching:

Efficiency equation:

$$\eta_{blc} = \frac{M_{43,k}}{M_{37,k}}; k \in K^{CONT}$$

Mass of disinfectant required for disinfection unit

$$M_{45,NaClO} = \Phi_{NaClO} \sum_{k \in K^{CONT}} M_{37,k}$$

Volume of disinfection unit:

$$Q_{dis} = V_{dis} = \theta_{dis}^R \left[\sum_{k \in K^s} \left(\frac{M_{37,k}}{\rho_k} \right) \right]$$

Power required for disinfection unit:

$$PW_{dis} = W_{sp_{dis}} Q_{dis}$$

Cost Model Equations

Stagewise Cost Equations

Annualized capital cost in each stage:

$$CCAC_{Nstg} = 1.66 \zeta_{RF} BMC_{mult} \sum_{i \in istg\{1,2,3,4\}} C_{ei}$$

Material Cost:

$$CCRM_{s1} = [\tau_{ann}(C_{pur_{Flcnt}})]$$

$$CCRM_{s2} = 0$$

$$CCRM_{s3} = [\tau_{ann}(C_{pur_{Lchrn}})]$$

$$CCRM_{s4} = [\tau_{ann}(C_{pur_{Oz}} + C_{pur_{NaClO}})]$$

Consumable Cost:

$$CCCS_{s1} = 0$$

$$CCCS_{s2} = Cons_{ftr}$$

$$CCCS_{s3} = Cons_{ads} + Cons_{mbrt}$$

$$CCCS_{s4} = Cons_{mbr}$$

Labor Cost

$$CCLC_{Nstg} = \tau_{ann} C_{Lab} \sum_{i \in istg\{1,2,3,4\}} Nlb_i$$

Utility Cost

$$CCUC_{Nstg} = \tau_{ann} C_{elec} \sum_{i \in istg\{1,2,3,4\}} PW_i$$

Other Cost

$$CCOC_{Nstg} = 2.78 \tau_{ann} C_{Lab} \sum_{i \in istg\{1,2,3,4\}} Nlb_i$$

Total Cost in each Stage

$$CCTC_{Nstg} = CCAC_{Nstg} + CCRM_{Nstg} + CCCS_{Nstg} + CCLC_{Nstg} + CCUC_{Nstg} + CCOC_{Nstg}$$

Total Category Cost:

$$CCTAC = \sum_{n \in Nstg\{1,2,3,4\}} CCAC_n$$

$$CCTRM = \sum_{n \in Nstg\{1,2,3,4\}} CCRM_n$$

$$CCTCS = \sum_{n \in Nstg\{1,2,3,4\}} CCCS_n$$

$$CCTL C = \sum_{n \in Nstg\{1,2,3,4\}} CCLC_n$$

$$CCTUC = \sum_{n \in Nstg\{1,2,3,4\}} CCUC_n$$

$$CCTOC = \sum_{n \in Nstg\{1,2,3,4\}} CCOC_n$$

$$CCTPC = CCTAC + CCTRM + CCTCS + CCTL C + CCTUC + CCTOC$$

Objective Function 1:

$$Obj = Min CCTPC$$

B.2 Model parameters and input data

Table B.2.1 Density and Molecular Weight of Components

Component	Value (kg/m ³)	Value (kg/kmol)
Water	1000	18
Solid particles	1800	102
Metals	2500	98
Chemicals	1100	48
Active pharmaceutical ingredient	1400	748.996
Ozone	2.14	48
Sodium Hypochlorite	1110	74.44
Flocculant	2200	2200
Liquid chlorine	1470	70.91

Table B.2.2 Purchase cost of added components

Component	Value (\$/kg)
Ozone	3.53
Sodium Hypochlorite	0.35
Flocculant	0.75
Liquid chlorine	2

Table B.2.3 Standard capacity, cost, laborers, and power for technologies

Unit Operation (costing capacity)	Standard Capacity (Units)	Standard Capacity Cost (million \$)	Standard Laborers Required (#/h)	Standard Power Required (kW/h)
Flocculation (Volume)	2000 (m ³)	0.538	0.1	0.0002
Filtration (Area)	80 (m ²)	0.039	0.5	0.1
Sedimentation (Volume)	2500 (m ³)	1.128	0.1	0.0002
Adsorption (Volume)	100 (m ³)	0.12	0.2	0.3
Membrane Bioreactor (Area)	40 (m ²)	1.194	0.1	0.2
Rotational Biological Container (Area)	185 (m ²)	0.045	0.3	0.01
Activated Sludge (Volume)	250 (m ³)	0.569	0.4	0.2
Disinfection (Volume)	540 (m ³)	0.627	0.7	0.5
Membrane Processes (Area)	80 (m ²)	0.938	0.5	0.2
Advanced Oxidation Processes (Volume)	1000 (m ³)	0.735	0.1	0.5
Bleaching (Volume)	500 (m ³)	0.100	0.5	0.33

Table B.2.4 Replacement time for technologies with consumables

Technology	Value (h/yr)
Filtration	2000
Adsorption	720
Membrane Processes	1000
Membrane Bioreactor	1000

Table B.2.5 Replacement cost for technologies with consumables

Technology	Value (\$/Unit)
Filtration	100
Adsorption	74.16
Membrane Processes	400
Membrane Bioreactor	400

B.2.6 Flocculation (flc):

Flocculent added (kg/kg) – 0.005

Residence time (h) – 0.5

B.2.7 Sedimentation (sdm):

Efficiency – 80%

Depth – 3m

B.2.8 Filtration (ftt):

Retention factor: Water – 0.05, Solids – 0.80, Metals – 0.10, Chemicals – 0.05, API – 0.50

Flux (m³/m².h): 0.2

B.2.9 Membrane Bioreactor (mbrt):

Retention factor: Water – 0.005, Solids – 0.95, Metals – 0.85, Chemicals – 0.50, API – 0.90
 Flux ($\text{m}^3/\text{m}^2\cdot\text{h}$): 0.025

B.2.10 Adsorption (ads):

Empty bed contact time (h): 0.25
 Density of granular activated carbon (GAC) (kg/m^3): 1030
 Efficiency: 90%
 Void fraction of GAC: 50%

B.2.11 Activated Sludge (asl):

Decay of biomass coefficient (h^{-1}): 0.0021
 Biomass yield (kg/kg): 0.5
 Hydraulic retention time (h): 2
 Efficiency: 80%

B.2.12 Rotating Biological Contactors (rbc):

Efficiency: 80%
 Hydraulic loading ($\text{m}^3/\text{m}^2\cdot\text{h}$): 20

B.2.13 Disinfection (dis):

Efficiency: 95%
 Ratio of liquid chlorine to contaminant (kg/kg): 0.00173
 Residence time (h): 2

B.2.14 Advanced Oxidation Processes (aop):

Ratio of ozone to contaminant (kg/kg): 0.000173
 Efficiency: 98%
 Residence time (h): 0.21

B.2.15 Membrane Processes (mbr):

Retention factor: Water – 0.05, Solids – 0.90, Metals – 0.90, Chemicals – 0.95, API – 0.95
 Flux ($\text{m}^3/\text{m}^2\cdot\text{h}$): 0.0856

B.2.16 Bleaching (blc):

Efficiency: 98%
 Ratio of sodium hypochlorite to contaminant (kg/kg): 0.00173
 Residence time (h): 2

B.3 Sustainable Process Index (SPI) Calculations**B.3.1 SPI for Municipal Wastewater Treatment****Parameters**

F_{RR} (kg/yr)	- feed of a processed resource (752400000)
y_R ($\text{kg}/\text{m}^2\cdot\text{yr}$)	- specific yield (243.1542)
$y_{EI,RN}$ ($\text{kWh}/\text{m}^2\cdot\text{yr}$)	- mean industrial energy yield or mean industrial energy supply density (7)
F_{RN} (kg/yr)	- feed of a processed resource (215463.6)[from GAMS Code]

C_N (\$/kg)	- price of the material (world market price, taxes excluded) (7)
C_E (\$/kWh)	- price of one kilowatt-hour of energy (industrial price, taxes excluded) (0.1)
F_E (kWh/yr)	- energy used in the process (450584.64)[from GAMS code]
y_E (kWh/m ² .yr)	- energy yield (43)
C_I (\$)	- total cost of energy for indirect installation (1329500)[from GAMS code]
LS (yr)	- depreciated area over the life-span years (30)
$y_{EI,II}$ (kWh/m ² .yr)	- industrial energy supply density or yield (43)
N_S (cap/yr)	- total number of workers in the treatment plant (80.19)
y_S (cap/m ² .yr)	- yield factor due to staff (3.59E-05)
$c_{c,m}$ (kg _m /kg)	- allowable concentration of substance, m [Solids, Chemical, Metals, Water] in the compartment, c [air, water, soil]
R_c (kg/m ² .yr)	- rate of renewal of the environmental compartments, c [air, water, soil]

Estimated Parameters

$E_{D,RN}$ - energy demand to supply one kilogram of the material in question for non-renewable energy (kWh/kg)

$$E_{D,RN} = \frac{0.95 C_N}{C_E} = \frac{0.95 \times 7}{0.1} = 66.5$$

$E_{D,II}$ - energy demand to supply one kilogram of the material in question for indirect land energy (kWh/yr)

$$E_{D,II} = \frac{0.54 C_I}{C_E \cdot LS} = \frac{0.54 \times 1329500}{0.1 \times 30} = 239310$$

$S_{c,m}$ - dissipation to potential sink (kg_m/m².yr)

$$S_{c,m} = R_c \cdot c_{c,m}$$

Analysis for R_{soil} (kg/m².yr)

Rate of soil renewal (RSN) in the US is 2.2E-04 m/yr

Assuming the soil is loamy with a 50% pore space, then the bulk density is 1330 kg/m³

$$R_{soil} = RSN \times Den_{bulk} = 0.00022 \times 1330 = 0.2926$$

Since we categorized contaminants into of solids, chemicals, and metals, we used contaminants that had the smallest allowable concentration for each category in the compartments to estimate S . For solids contaminant, we used lead (Pb), for chemical we used Chromium (Cr), and for metals we used lead (Pb).

Analysis for $S_{soil,m}$ (kg_m/m².yr)

$$S_{soil,m} = R_{soil} \cdot c_{soil,m}$$

Component (m)	C _(soil,m) (kgm/kg)	S _(soil,m) (kgm/m ² .y)
Solids (Sslds)	1.00E+00	2.93E-01
Chemical (Chem)	1.00E-04	2.93E-05
Metals (Mtls)	2.00E-06	5.85E-07
Water (Wtr)	1.00E+00	2.93E-01
API	1.00E-04	2.93E-05

Analysis for R_{water} (kg/m².yr)

Average rate of precipitation (RP) form Jan, 2009 to Dec, 2019 in the US is 31.91 in/yr (0.810514 m/yr)

Seeping ratio (SR) of water is 0.30

$$R_{water} = RP \times SR \times Den_{water} = 0.810514 \times 0.30 \times 1000 = 243.1542$$

Analysis for S_{water,m} (kgm/m².yr)

Component (m)	C _(water,m) (kgm/kg)	S _(water,m) (kgm/m ² .y)
Solids (Sslds)	1.67E-06	4.05E-04
Chemical (Chem)	1.00E-07	2.43E-05
Metals (Mtls)	1.50E-08	3.65E-06
Water (Wtr)	1.00E+00	2.43E+02
API	1.00E-07	2.43E-05

$$S_{air,chem} \text{ (kgm/m}^2\text{.yr)} = 6.50E-03$$

FP_{c,m} product flow rate to compartment c, by substance, m (kg_m/yr) [from GAMS code]

Component (m)	Fraction of m into compartment c			FP _{c,m}		
	Air	Water	Soil	Air	Water	Soil
Solids (Sslds)	0	0.05	0.95	0.00E+00	7.92E+03	1.50E+05
Chemical (Chem)	0.03	0.9	0.07	9.93E+04	2.98E+06	2.32E+05
Metals (Mtls)	0	0.7	0.3	0.00E+00	4.99E+02	2.14E+02
Water (Wtr)	0	0.95	0.05	0.00E+00	7.15E+08	3.76E+07
API	0	0.5	0.5	0.00E+00	7.92E+03	7.92E+03

Variables

A_R - area for raw material production (m²/yr)

A_{RR} - area for renewable raw material production (m²/yr)

A_E - area for energy production (m²/yr)

A_I - area for installation for equipment and other infrastructure (m²/yr)

A_{ID} - area for direct installation (m²/yr)

A_{II} - area for indirect installation (m²/yr)

A_S - area for staff (m²/yr)

A_{P,c,m} - area for dissipating a single component of particular product flow to a given compartment (m²/yr)

A_{PS,c} - area assined to the dissipation of a particular product stream, S (m²/yr)

A_P - area for product dissipation (m²/yr)

A_{tot} - total area (m²/m³WW-yr)

Area for Raw Material Production (A_R)

Area for Renewable Raw Material Production (A_{RR})

$$A_{RR} = \frac{F_{RR}}{y_R} = \frac{7524000000}{243.1542} = 3.09E06$$

Area for Non-Renewable Raw Material Production (A_{RN})

$$A_{RN} = \frac{F_{RN} \cdot E_{D,RN}}{y_{EI,RN}} = \frac{0 \times 66.5}{7} = 0$$

$$A_R = A_{RR} + A_{RN} = 3.09E06$$

Area for Energy Production (A_E)

$$A_E = \frac{F_E}{y_E} = \frac{450584.64}{43} = 1.05E4$$

Area for Installations (A_I)

$$A_I = A_{ID} + A_{II}$$

Area for Direct Installation (A_{ID})[from GAMS Code]

Flocculation technology = 17.43

Filtration technology = 494.63

Adsorption technology = 4.95

$$A_{ID} = 517.00$$

Area for Indirect Installation (A_{II})

$$A_{II} = \frac{E_{D,II}}{y_{EI,II}} = \frac{239310}{43} = 5.57E3$$

Area for Staff (A_S)

$$A_S = N_S \cdot a_{in} = \frac{N_S}{y_S} = \frac{1037.19}{0.000035} = 2.89E7$$

Area for Product Dissipation into Various Environmental Compartment (A_P)

$$A_{P,c,m} = \frac{F_{P,c,m}}{S_{c,m}}$$

Component (m)	AP,c,m		
	Air	Water	Soil
Solids (Sslds)	--	1.95E+07	5.14E+05
Chemical (Chem)	1.53E+07	1.23E+11	7.92E+09
Metals (Mtls)	--	1.37E+08	3.65E+08
Water (Wtr)	--	2.94E+06	1.29E+08
API	--	3.26E+08	2.71E+08

$$A_{PS,c} = \max_m(A_{P,c,m})$$

Highlighted are the maximum values for each component

Component (m)	AP,c,m		
	Air	Water	Soil
Solids (Sslds)	--	1.95E+07	5.14E+05
Chemical (Chem)	1.53E+07	1.23E+11	7.92E+09
Metals (Mtls)	--	1.37E+08	3.65E+08
Water (Wtr)	--	2.94E+06	1.29E+08
API	--	3.26E+08	2.71E+08

$$A_P = \sum_c A_{PS,c} = 1.30E11$$

$$A_{tot} = A_R + A_E + A_I + A_S + A_P = 1.30E+11 \text{ m}^2/\text{yr} = 1.65E+05 \text{ (m}^2/\text{m}^3\text{WW-yr)}$$

B.3.1 SPI for Direct Disposal of Pharmaceutical Wastewater

We considered on the area needed to sustainably embed the wastewater into the ecosystem, i.e. A_P

Area for Product Dissipation into Various Environmental Compartment (A_P)

F_{P,c,m} product flow rate to compartment c, by substance, m (kg_m/yr) [from GAMS code]

Component (m)	Fraction of		F _{P,c,m}	
	Water	Soil	Water	Soil
Solids (Sslds)	0.05	0.95	4.38E+05	8.32E+06
Chemical (Chem)	0.95	0.05	3.66E+07	1.93E+06
Metals (Mtls)	0.7	0.3	6.13E+03	2.63E+03
Water (Wtr)	0.95	0.05	8.32E+08	4.38E+07
API	0.5	0.5	1.75E+05	1.75E+05

$$A_{P,c,m} = \frac{F_{P,c,m}}{S_{c,m}}$$

Component (m)	AP,c,m	
	Water	Soil
Solids (Sslds)	1.08E+09	2.84E+07
Chemical (Chem)	1.51E+12	6.59E+10
Metals (Mtls)	1.68E+09	4.49E+09
Water (Wtr)	3.42E+06	1.50E+08
API	7.21E+09	5.99E+09

$$A_{PS,c} = \max_m(A_{P,c,m})$$

Highlighted are the maximum values for each component

Component (m)	$A_{P,c,m}$	
	Water	Soil
Solids (Sslds)	1.08E+09	2.84E+07
Chemical (Chem)	1.51E+12	6.59E+10
Metals (Mtls)	1.68E+09	4.49E+09
Water (Wtr)	3.42E+06	1.50E+08
API	7.21E+09	5.99E+09

$$A_P = \sum_c A_{PS,c} = 1.57E12$$

$$A_{tot} = A_P = 1.57E+12 \text{ m}^2/\text{yr} = 1.79E+06 \text{ (m}^2/\text{m}^3\text{WW-yr)}$$