NYWEA MEMBER EDUCATION VIRTUAL TRAINING

SIMULATION OF WASTEWATER TREATMENT PROCESSES

May 4, 2021

Mark Greene, Ph.D.



AGENDA

Purpose and Procedure
Data Analysis
Influent Characterization
Model Building
Simulations

PURPOSE OF MODELING

Intended uses

- Design for retrofit or new plant
- Process optimization



Evaluate plant performance



 Evaluate different operating conditions



Additional Benefits





 Alternative/precursor to pilot testing



- Support, develop, and refine design decisions
- Translate results to real world solutions





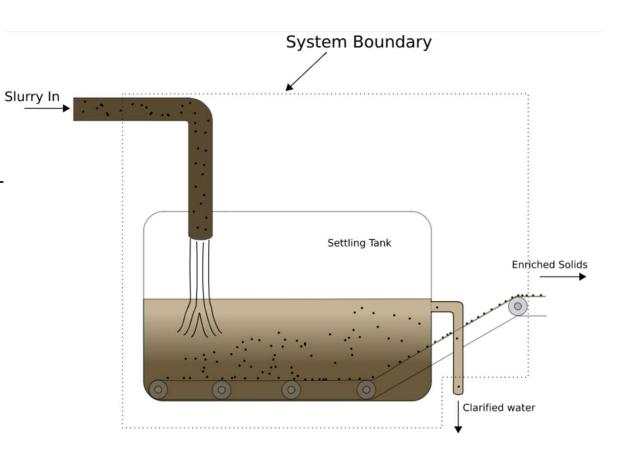
WHAT IS MODELING?

Mass Balance

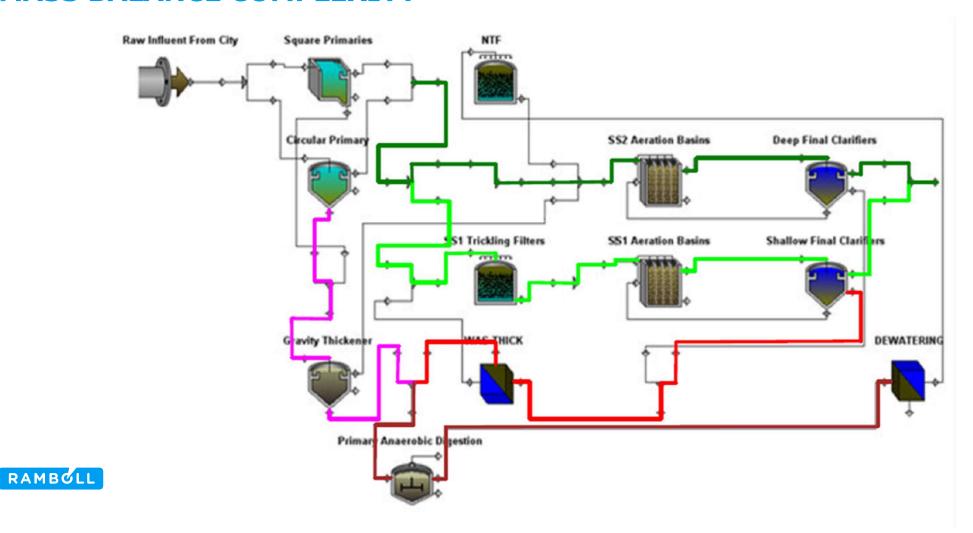
Input + Generation =

Output + Accumulation +

Consumption



MASS BALANCE COMPLEXITY



PROCESS MODELING SOFTWARE

 Differences in modeling software are like differences in "Calculator" models (Casio vs Texas Instruments)

- Minor variations in model implementation
 - Dynamic vs Static Modeling
 - Kinetic/Stoichiometric parameters
 - Model outputs
 - Computation speed
 - Output variables



AQUIFAS+







IWA GUIDELINES FOR USE OF ACTIVATED SLUDGE COMPUTER MODELS

Unified protocol for wastewater modeling:

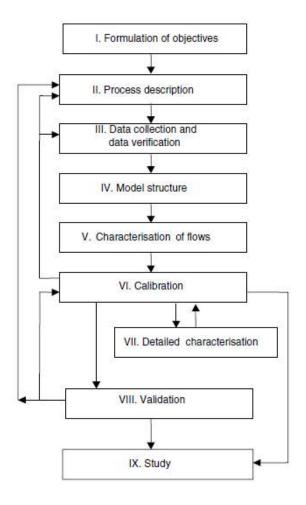
- 1. Project definition
- 2. Data collection and reconciliation
- 3. Model set-up
- 4. Calibration and validation
- 5. Simulation and results interpretation



Task Group on Good Modelling Practice (gmp)



Guidelines for use of activated sludge models



GARBAGE IN = GARBAGE OUT

- Influent characterization
- Recycle and side stream characterization
- Basin sizes
- Biological kinetics
- Calibration parameters
 - MLSS
 - Effluent quality
 - Sludge production
- Solids handling impacts are critical,
 - Especially with anaerobic digestion

99-WWF-3 (2003)

Treatment Processes and Systems



Methods for Wastewater
Characterization in Activated
Sludge Modeling

Co-published by





QUESTION 1

Why use models?

- a. Saves money
- b. Good way to see the impact of process changes
- c. Quick way to get answers
- d. All of the above
- e. None of the above

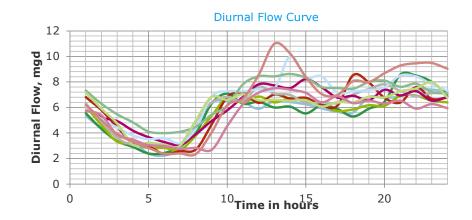


AGENDA

01	Purpose and Procedure
02	Data Analysis
03	Influent Characterization
04	Model Building
05	Simulations

DATA ANALYSIS

- Influent flow, loads
- Infiltration and Inflow
- Peak flow conditions
- Diurnal flow conditions
- Influent characterization
 - BOD/COD, COD/TKN, and COD/TP ratios
 - VSS/TSS
- Municipal vs Industrial
- Impact of recycles



Ratio	Units	Typical Range
VSS / TSS	gVSS/gTSS	0.6 - 0.85
BOD₅/COD	gBOD ₅ /gCOD	0.4 - 0.55
NH₄-N / TKN	-	0.65 - 0.9
Filtered COD / Total COD		0.25 – 0.7

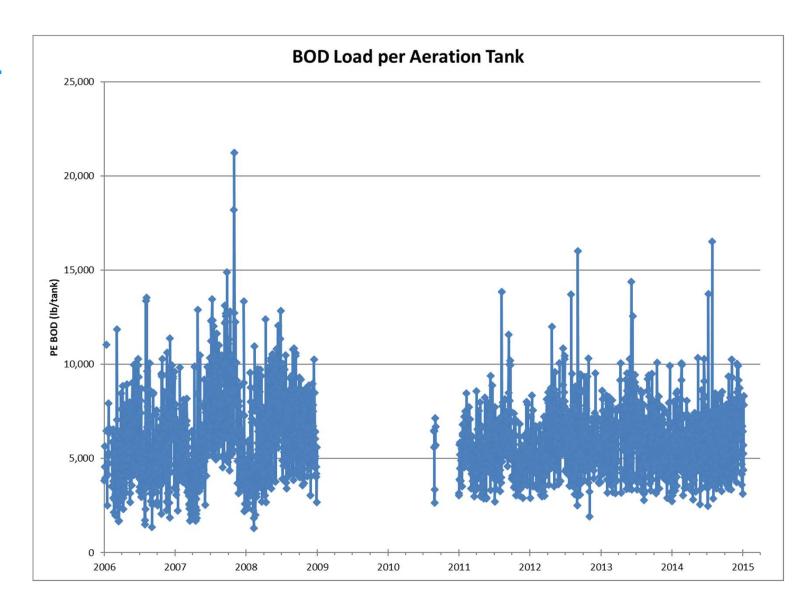
Min. ratios for Nutrient Removal: BOD/TKN = 4 and BOD/TP = 20



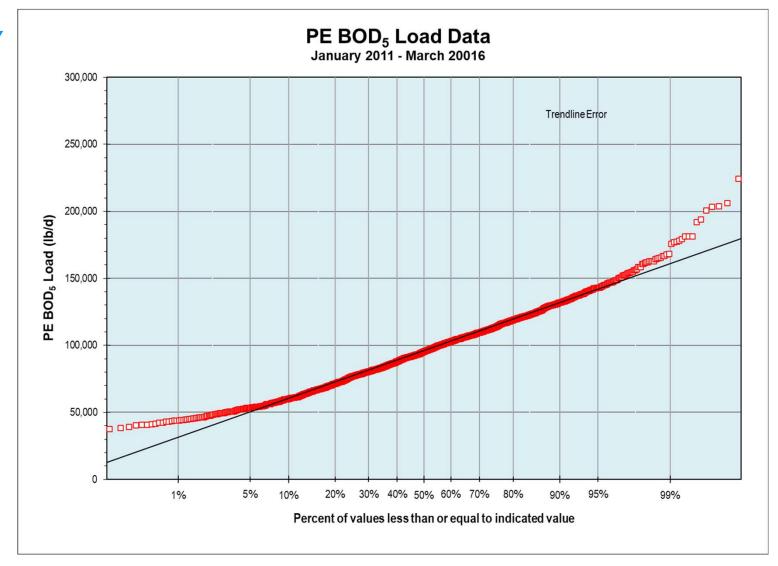
PROCESS DATA

- 4	Α	В	C	D	E	F	G	Н	1	J	K	L	M	0
1	Date	Eff	Prim Eff	PE BOD	PE BOD	PE BOD	PE BOD	Aeration	Aeration	Aeration	MLSS	MLVSS	SSV 30	SVI
2		Flow	mon avg	8031	mon avg	Load	mon avg	BOD Load	F:M	Mass	7128	7129		7109
3	▼.	MGD 💌	MGD 🕶	mg/L ▼	mg/L ▼	ppd ▼	ppd 🔻	lb/kcf/(▼	lb/lb/c ▼	lb ▼	mg/L ▼	mg/L ▼	ml/L 💌	ml/g ▼
3325	12/19/2014	86		137		98,262		70	0.77	128,000	1,470		115	78
3326	12/20/2014	81								114,000	1,310		120	92
3327	12/21/2014	80		113		75,394		54	0.62	121,000	1,390		130	94
3328	12/22/2014	76		145		91,907		66	0.69	133,000	1,520		150	99
3329	12/23/2014	86		168		120,496		86	0.76	158,000	1,810		160	88
3330	12/24/2014	86								139,000	1,590		160	101
3331	12/25/2014													
3332	12/26/2014	72		117		70,256		50	0.58	121,000	1,390		140	101
3333	12/27/2014	71		91		53,885		38	0.42	129,000	1,480		140	95
3334	12/28/2014	74		101		62,333		45	0.48	131,000	1,500		150	100
3335	12/29/2014	72		168		100,881		72	0.70	144,000	1,650		180	109
3336	12/30/2014	70	_							165,000	1,890		210	111
3337	12/31/2014	71	81	174		103,032		69	0.66	156,000	1,680		200	119
3393														
3401	11/2011 to 1/2	015												
3402	Average	88	88	141	140	97,072	97,359	62	0.57	179,000	1,801		241	134
3403			_											
3404	Maximum	504	132	298	173	231,185	121,558	173	2.34	359,000	2,960		820	425
3405	Median	79	86	140	143	96,077	94,471	62	0.54	172,000	1,790		230	129
3406	Minimum	46	64	49	90	32,559	79,022	20	0.17	78,000	870		80	55
3407														
3408	Count	1,187	38	1,009	36	1,009	36	1,007	1,007	1,185	1,185	0	1,175	1,173
3409														

HISTORICAL TRENDS



PROBABILITY PLOT





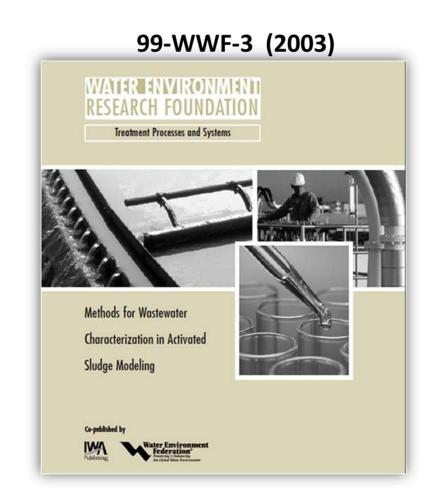
AGENDA

01	Purpose and Procedure
02	Data Analysis
03	Influent Characterization
04	Model Building

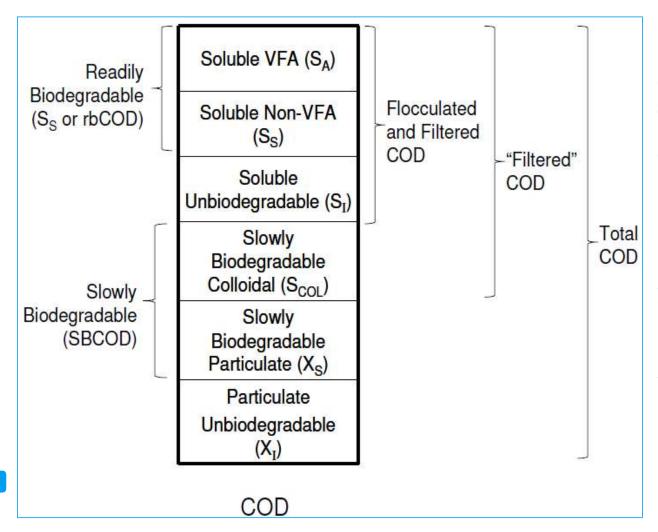
INFLUENT CHARACTERISTICS

- Key activity to develop a representative and robust model
- Influent characterization needs are not part of the typical sampling protocol
- Additional sampling may be required to gain better understanding of site-specific values
- Uncommon parameters
 - COD, TKN
 - Soluble fractions
 - Readily biodegradable
 - Slowly biodegradable





INFLUENT CHARACTERIZATION - COD



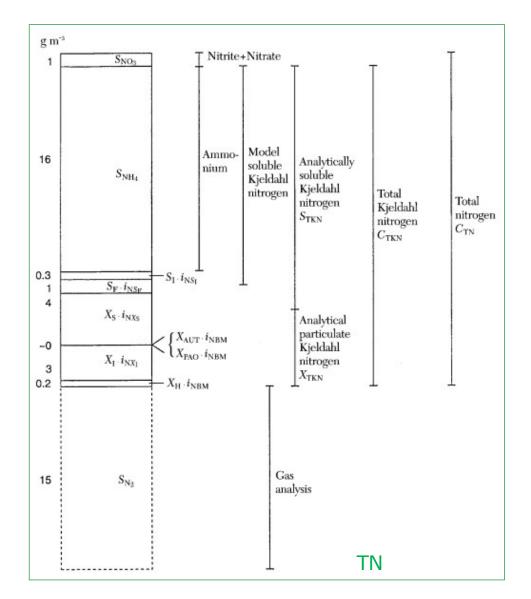
Routine sampling includes BOD and COD but not the soluble and particulate fractions of COD

"Filtered" COD is measured by filtering through a glass fiber, 1.2 µm filter and analyzing the filtrate.

"Flocculated and Filtered" COD is measured by flocculating the wastewater sample with Zn(OH)2 at pH=10.5 and filtering with a 0.45 μm filter, then analyzing the filtrate.

TOTAL NITROGEN

Typically ammonium and TKN are measured

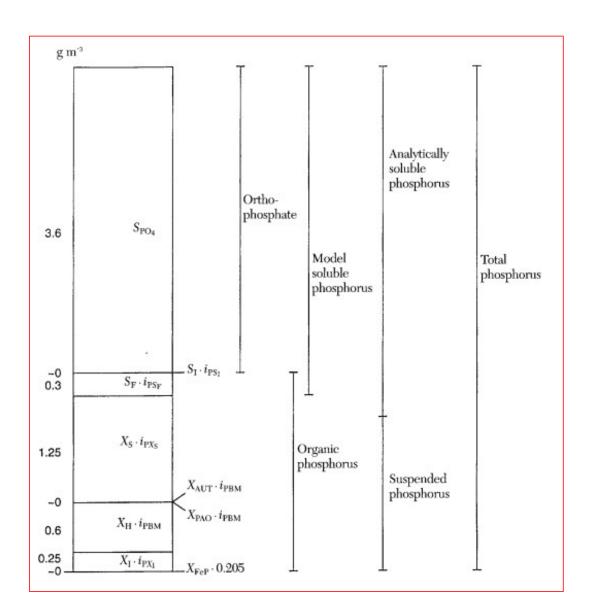


TOTAL PHOSPHORUS

Usually Total Phosphorus is measured

Ortho-Phosphate may not be part of routine sampling





BIOWIN INFLUENT SPECIFIER

Measurements	Value	Unit
Main influent concentrations		
Flow	0.4	mgd or m3/d
Total COD	4096.0	mgCOD/L
Total Kjeldahl Nitrogen	202.0	mgN/L
Total P	154.0	mgP/L
Other influent concentrations		0.25
Nitrate N	4.6	mgN/L
рН	6.8	
Alkalinity (CaCO3 equivalent)	998.0	mgCaCO3/L
Calcium	300.0	mg/L
Magnesium	300.0	mg/L
Dissolved oxygen	1.0	mgO2/L
Other measurements		
Effluent filtered COD	60.0	mgCOD/L
Influent filtered COD (GFC)	1966.0	mgCOD/L
Influent FF COD	1065.0	mgCOD/L
Influent acetate	100.0	mgCOD/L
Influent ammonia	24.0	mgN/L
Influent ortho-phosphate	96.0	mgP/L
Influent carbonaceous BOD5	2223.0	mgO2/L
Influent filtered cBOD5	956.0	mgO2/L
Influent VSS	2314.0	mgVSS/L
Influent TSS	2612.0	mgTSS/L

GUIDE

Enter measured lab data in column on left (BOLD)
 (If data is missing, estimate. May need to repeat after Step 2)
 Check resulting fractions (BOLD)

Parameter	Value	Unit	Typical range
Alkalinity (molar)	20.0	meq/L	2 - 6
Fus	0.01		0.03 - 0.08
CODp	2130.0	mgCOD/L	
Fbs	0.25	-	0.12 - 0.25
Fac	0.10	-	0.0 - 0.3
Fna	0.12	-	0.5 - 0.8
Fpo4	0.62	-	0.3 - 0.6
COD/BOD5	1.84	2	1.9 - 2.2
Fcv	0.92	mgCODp/mgVSS	1.5 - 1.7
ISS	298.0	mgISS/L	15 - 45

ESTIMATE COD FRACTIONS (STEP 2)

Change F_{up},

F_{xsp} to

achieve

Excellent

Match Status

Influent COD fractions	Default	Estimate	Notes
Fbs	0.160	0.246	from Step 1
Fus	0.050	0.014	from Step 1
Fup	0.130	0.200	affects BOD, VSS
Fzbh	0.000	0.000	from separate method
Fxs	0.660	0.540	by difference (must be > 0!!)
Fxsp	0.750	0.600	affects VSS, scale: 0 to 1

Influent values	Measured (From Step 1)	Calculated (Based on	Match Status
L. L.	1	fractions above)	
CODt	4096	4096	Excellent
Soluble COD (GFC)	1966	1950	Excellent
FF COD	1065	1065	Excellent
cBOD5	2223	2037	Acceptable
fcBOD5	956	1336	Unacceptable
VSS	2314	2332	Excellent
TSS	2612	2630	Excellent

Calculated cond Sus	,	59	1.17 (200.00 (17.01))
Xi	•	819	
Sbs	•	1007	
Xs (c+p)		2212	
Zbh	•	0	
Xsc		885	Added to Ss for BOD calcs
Xsp	•	1327	

GUIDE

- Change COD fractions (BOLD) until match is achieved

Suggestion:

Inhibited cBOD5 = 0.84 x "true" cBOD5

Important fractions	(can be used as a check)			
Fraction	Value	Typical range		
COD/cBOD5	2.01	1.9-2.2		
Sol. COD fraction	0.48	0.3-0.5		
VSS/TSS	0.89	0.75-0.85		

RAMBOLL

1

BIOWIN STEP 3 – CUT AND PASTE

COD Influent data

Name	Value
Flow	0.368
Total COD mg/L	4096
Total Kjeldahl Nitrogen mgN/L	202
Total P mgP/L	154
Nitrate N mgN/L	4.6
pH	6.8
Alkalinity mmol/L	19.96
Inorganic S.S. mgTSS/L	298.0
Calcium mg/L	300
Magnesium mg/L	300
Dissolved oxygen mg/L	1

$Project \rightarrow Parameters \rightarrow Other \rightarrow General$

Particulate substrate COD:VSS ratio	0.92
Particulate inert COD:VSS ratio	0.92

COD Influent fractions

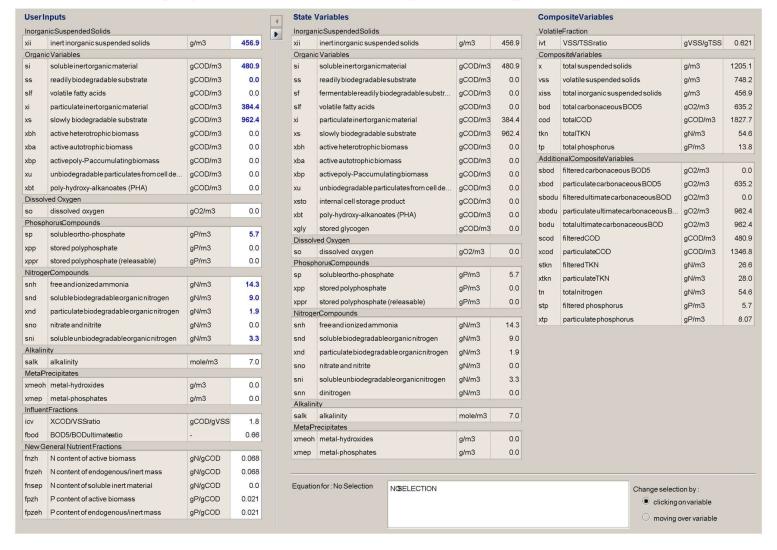
Name	Raw defaults	Value
Fbs - Readily biodegradable (including Acetate) [gCOD/g of total COD]	0.16	0.246
Fac - Acetate [gCOD/g of readily biodegradable COD]	0.15	0.099
Fxsp - Non-colloidal slowly biodegradable [gCOD/g of slowly degradable COD	0.75	0.600
Fus - Unbiodegradable soluble [gCOD/g of total COD]	0.05	0.014
Fup - Unbiodegradable particulate [gCOD/g of total COD]	0.13	0.200
Fna - Ammonia [gNH3-N/gTKN]	0.66	0.119
Fnox - Particulate organic nitrogen [gN/g Organic N]	0.5	0.500
Fnus - Soluble unbiodegradable TKN [gN/gTKN]	0.02	0.020
FupN - N:COD ratio for unbiodegradable part. COD [gN/gCOD]	0.035	0.035
Fpo4 - Phosphate [gPO4-P/gTP]	0.5	0.623
FupP - P:COD ratio for influent unbiodegradable part. COD [gP/gCOD]	0.011	0.011
FZbh - Non-poly-P heterotrophs [gCOD/g of total COD]	1.00E-04	0.0001
FZbm - Anoxic methanol utilizers [gCOD/g of total COD]	1.00E-04	0.0001
FZaob - Ammonia oxidizers [gCOD/g of total COD]	1.00E-04	0.0001
FZnob - Nitrite oxidizers [gCOD/g of total COD]	1.00E-04	0.0001
FZamob - Anaerobic ammonia oxidizers [gCOD/g of total COD]	1.00E-04	0.0001
FZbp - PAOs [gCOD/g of total COD]	1.00E-04	0.0001
FZbpa - Propionic acetogens [gCOD/g of total COD]	1.00E-04	0.0001
FZbam - Acetoclastic methanogens [gCOD/g of total COD]	1.00E-04	0.0001
FZbhm - H2-utilizing methanogens [gCOD/g of total COD]	1.00E-04	0.0001

GUIDE

Paste data from this page to the two influent forms and the parameter form in BioWin

GPS -X INFLUENT ADVISOR

Influent Advisor - Library: cnplib - Influent Model: states - Biological Model: newgeneral





SPECIAL SAMPLING PROGRAM-INFLUENT ADVISOR EXAMPLE

	total carbonaceous BOD5	gO2/m3	230.0
×	total suspended solids	g/m3	240.0
tkn	total TKN	gN/m3	40.0
Organ	ic Variables		22
si	soluble inert organic material	gCOD/m3	21.5
slf	volatile fatty acids	gCOD/m3	0.0
xbh	active heterotrophic biomass	gCOD/m3	0.0
xba	active autotrophic biomass	gCOD/m3	0.0
xbp	active poly-P accumulating biomass	gCOD/m3	0.0
xbt	poly-hydroxy-alkanoates (PHA)	gCOD/m3	0.0
Dissol	ved Oxygen		
so	dissolved oxygen	gO2/m3	0.0
Phosp	horus Compounds		
sp	soluble ortho-phosphate	gP/m3	5.9
хрр	stored polyphosphate	gP/m3	0.0
Nitrog	en Compounds	i e	100
sno	nitrate and nitrite	gN/m3	0.0
snn	dinitrogen	gN/m3	0.0
Alkalin	nity		

User Input Values

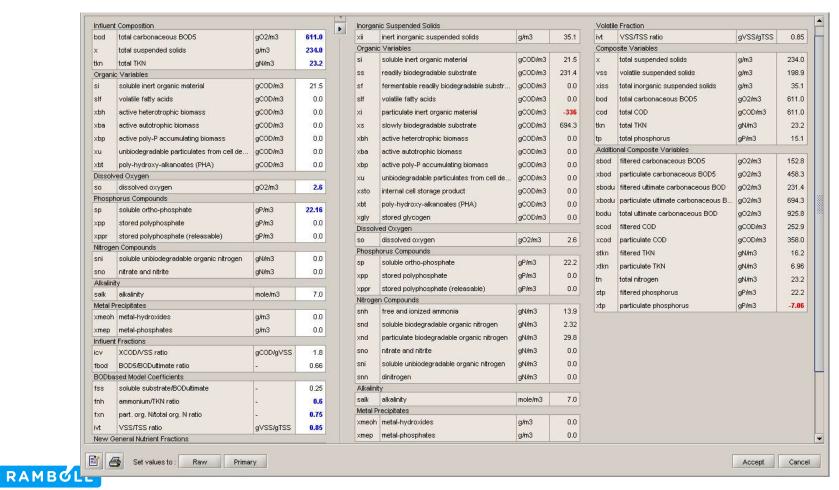
Used to Calculate other parameters

• Raw inf. and Primary Eff. defaults

Soluble and Special Sampling parameters



SPECIAL SAMPLING PROGRAM- INFLUENT ADVISOR EXAMPLE



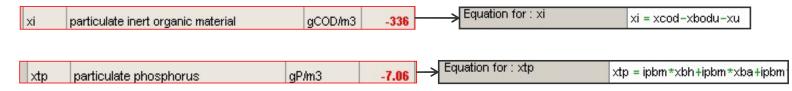
SPECIAL SAMPLING PROGRAM- INFLUENT ADVISOR EXAMPLE

bod	total carbonaceous BOD5	gO2/m3	611.0
x	total suspended solids	g/m3	234.0
tkn	total TKN	gN/m3	23.2
Organ	ic Variables		100
si	soluble inert organic material	gCOD/m3	21.5
slf	volatile fatty acids	gCOD/m3	0.0
xbh	active heterotrophic biomass	gCOD/m3	0.0
xba	active autotrophic biomass	gCOD/m3	0.0
xbp	active poly-P accumulating biomass	gCOD/m3	0.0
xu	unbiodegradable particulates from cell de	gCOD/m3	0.0
×bt	poly-hydroxy-alkanoates (PHA)	gCOD/m3	0.0
Dissol	ved Oxygen	Legisland Control of the Control of	
so	dissolved oxygen	gO2/m3	2.6
Phosp	horus Compounds	÷.	
sp	soluble ortho-phosphate	gP/m3	22.16

Blue Text shows input parameters

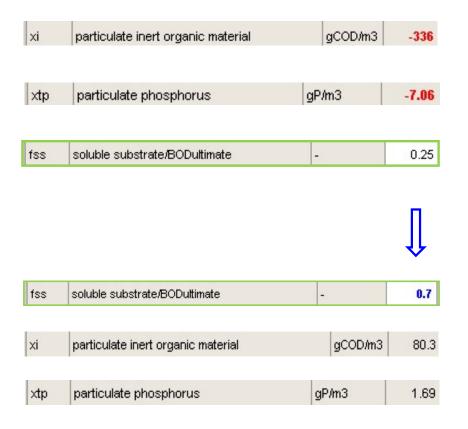
Red Text shows negative values

Clicking on Calculated values shows variables and equations used





SPECIAL SAMPLING PROGRAM- INFLUENT ADVISOR EXAMPLE



 Both negative values were calculated using the soluble BOD fraction

 Changing this ratio from default to existing conditions...

... allows parameters to be calculated realistically.



QUESTION 2

How does one characterize your influent wastewater?

- a. Collect existing data
- b. Collect special samples
- c. Depends on the purpose
- d. All of the above



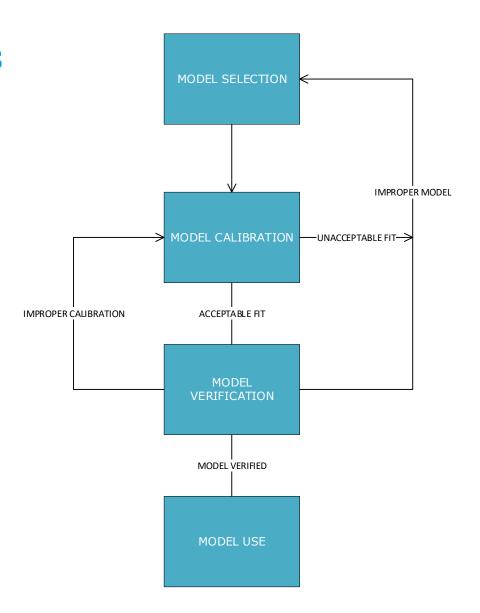
AGENDA

05	Simulations
04	Model Building
03	Influent Characterization
02	Data Analysis
01	Purpose and Procedure

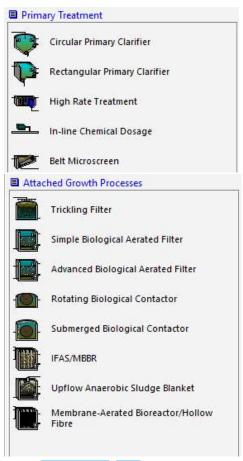
MODEL DEVELOPMENT STEPS

- Calibrate to average data
 - 3-year period
 - 5-year period
- Validate to a time period
 - Warm weather
 - Cold weather
 - An individual month

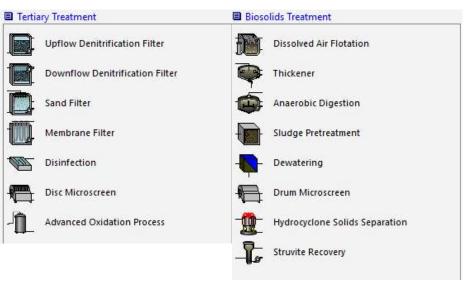




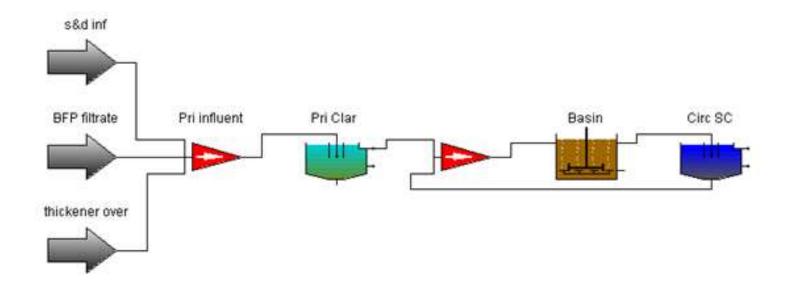
GPS-X TREATMENT UNITS





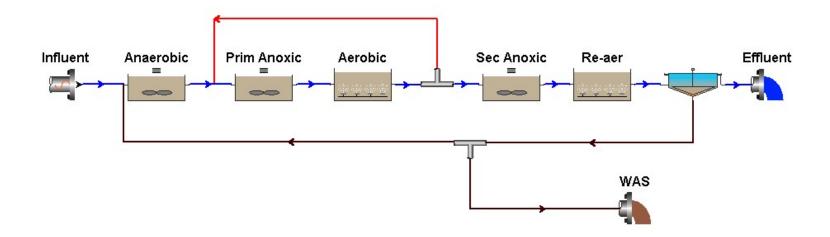


SIMPLE PRIMARY-SECONDARY PROCESS FLOWSHEET





BIOLOGICAL NUTRIENT REMOVAL FLOWSHEET





MODEL CALIBRATION

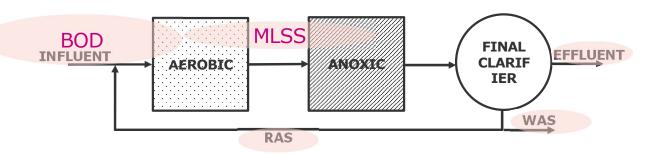
- Model calibration objective is to minimize the error between actual data and model prediction
- Establish a field of validity for the model
- Goal is to match as many measured key performance variables as reasonably as possible
- Select model accuracy depending on the specific conditions
- Compare the model prediction to "conditioned" actual data
- Calibration levels:
 - Level 1 Defaults and assumptions only
 - Level 2 Historical data only
 - Level 3 Full-Scale testing
 - Level 4 Direct Parameter measurements





KEY PROCESS PERFORMANCE VARIABLES

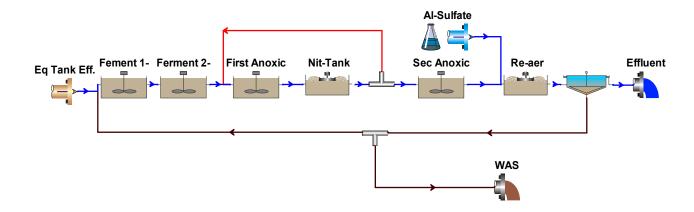
- Solids yield = Ib TSS generated/Ib BOD influent
- Food to microorganism ratio = Ib BOD in /Ib MLSS in the reactor
- Solids retention time = lb MLSS in the reactor/lb/d waste solids (aerobic SRT)
- MLVSS/MLSS
- Effluent performance
 - BOD, TSS
 - NH3-N, NOx, TKN
 - Ortho-P, TP



Match key performance variables observed with model values at given temperature



EXAMPLE- MODEL CALIBRATION OF 5-STAGE PROCESS



- Level 2 Calibration
- 5-stage
- SRT = 40 days
- IR = 3.5 Q, RAS = Q
- Alum = 140 gpd
- MLSS ~ 6,600 mg/L



Based on Average of Sept. 2007 Data	Eq Tank Eff.
Flow	0.48
Total Carbonaceous BOD mgBOD/L	196.00
Volatile suspended solids mgVSS/L	105.00
Total suspended solids mgTSS/L	141.00
Total Kjeldahl Nitrogen mgN/L	35.00
Total P mgP/L	6.70
Nitrate N mgN/L	0
рН	7.30
Alkalinity mmol/L	6.00
Calcium mg/L	80.00
Magnesium mg/L	15.00
Dissolved oxygen mg/L	0

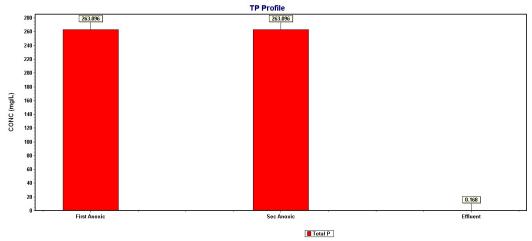
MODEL PARAMETERS

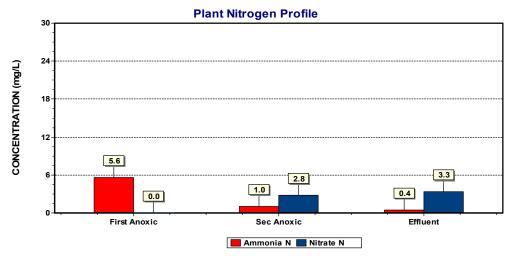
Model Parameters	Eq Tank Eff.	Default
Fbs - Readily biodegradable (including Acetate) [gCOD/g of	0.16	
total COD]		0.16
Fac - Acetate [gCOD/g of readily biodegradable COD]	0.15	0.15
Fxsp - Non-colloidal slowly biodegradable [gCOD/g of slowly degradable COD]	0.4810	0.75
Fus - Unbiodegradable soluble [gCOD/g of total COD]	0.05	0.05
Fup - Unbiodegradable particulate [gCOD/g of total COD]	0.13	0.13
Fna - Ammonia [gNH3-N/gTKN]	0.66	0.66
Fnox - Particulate organic nitrogen [gN/g Organic N]	0	0.5
Fnus - Soluble unbiodegradable TKN [gN/gTKN]	0	0.02
FupN - N:COD ratio for unbiodegradable part. COD [gN/gCOD]	0.0350	0.035
Fpo4 - Phosphate [gPO4-P/gTP]	0.5	0.5
FupP - P:COD ratio for influent unbiodegradable part. COD	0.011	
[gP/gCOD]		0.011
FZbh - Non-poly-P heterotrophs [gCOD/g of total COD]	0.0001	1.00E-04
FZbm - Anoxic methanol utilizers [gCOD/g of total COD]	0.0001	1.00E-04
FZaob - Ammonia oxidizers [gCOD/g of total COD]	0.0001	1.00E-04
FZnob - Nitrite oxidizers [gCOD/g of total COD]	0.0001	1.00E-04
FZamob - Anaerobic ammonia oxidizers [gCOD/g of total COD]	0.0001	1.00E-04
FZbp - PAOs [gCOD/g of total COD]	0.0001	1.00E-04
FZbpa - Propionic acetogens [gCOD/g of total COD]	0.0001	1.00E-04
FZbam - Acetoclastic methanogens [gCOD/g of total COD]	0.0001	1.00E-04
FZbhm - H2-utilizing methanogens [gCOD/g of total COD]	0.0001	1.00E-04



CALIBRATION SUMMARY

Parameter	Actual (Average)	Model
Plant Eff. NH3 (mg-N/L)	0.0 - 0.3	0.4
Plant Eff. NOx (mg-N/L)	1.8 - 2.5	3.3
Plant Eff. Org-N (mg-N/L)	0.7 - 1.0	1.3
Plant Eff. TN (mg-N/L)	2.5 - 3.8	5.0
Plant Eff. TP (mg-P/L)	0.06 - 0.15	0.17
DO in aeration zone (mg/L)	0.1 - 1.0	0.5
MLSS (mg/L)	6,120 - 9,390	6,600
Alum dosage (gpd)	140	140
Temperature (°F)	44-77	59

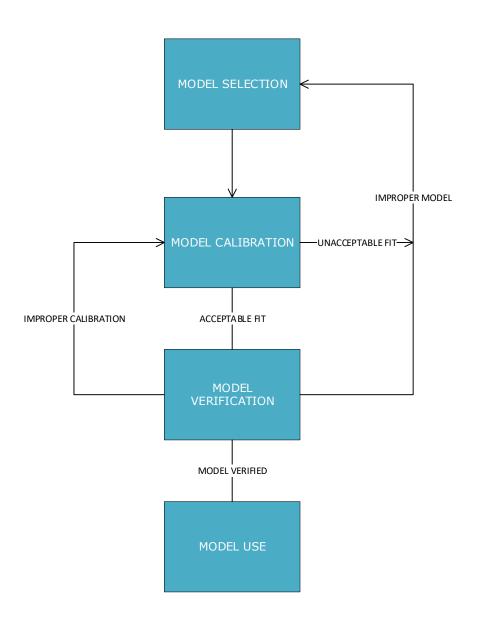






VALIDATION/VERIFICATION

- Same activity as calibration
 - Using a different set of data for input values
 - Using the different set of data for comparing key performance values
- If you "tweak" the model based on validation results
 - Repeat the calibration





QUESTION 3

Why bother to calibrate my model?

- a. So the results can be reliable
- b. It is too complicated, tedious and confusing
- c. The model cannot achieve an exact match with the performance on my treatment plant
- d. Because once you calibrate a model, you have to do more work to validate it



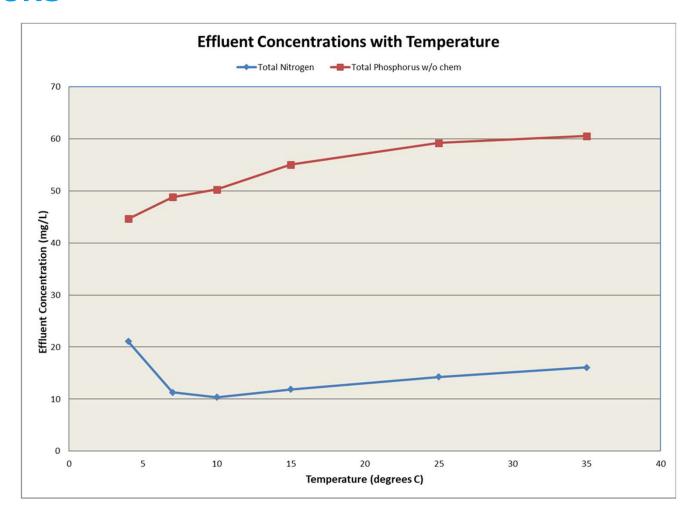
AGENDA

05	Simulations
04	Model Building
03	Influent Characterization
02	Data Analysis
01	Purpose and Procedure

RAMBOLL

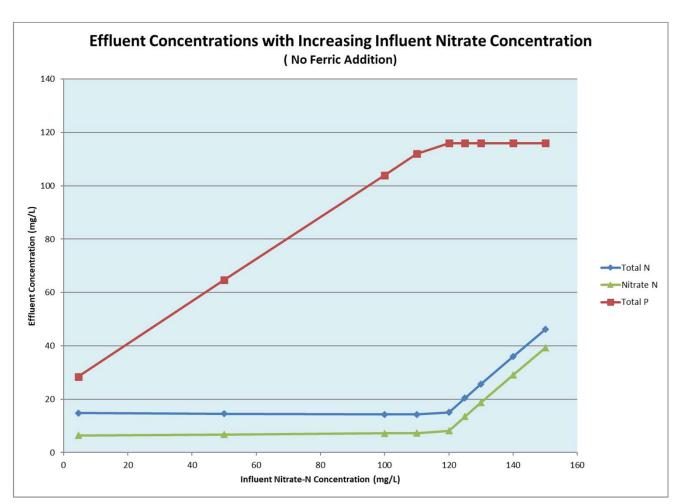
VARIABLE CONDITIONS

- Design Basis
 - Annual Average
 - Monthly Maximum
 - Peak Day
- Future Growth
- Seasonal Temperatures
- Wet Weather
- Equipment out of service



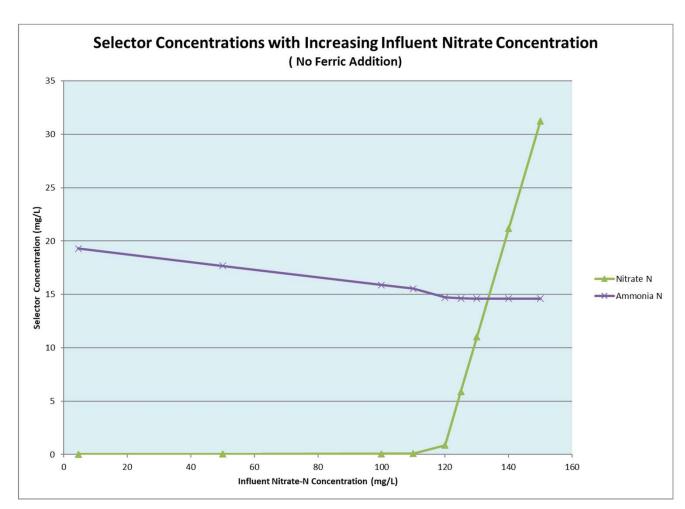


INFLUENT NITRATE





INFLUENT NITRATE





SENSITIVITY ANALYSIS

- Run static model in dynamic mode
 - Diurnal patterns/impacts
 - Impacts of slug loads/wet weather flow
- Split a complex model into smaller pieces
 - Quicker simulations with more work to combine the results
- Evaluate the impact of changing operating conditions
 - Higher/lower internal recycle rates for BNR
 - Longer/shorter sludge age



SENSITIVITY

Trials 4,5:
lowest
effluent
COD, TKN,
highest TP

Trial **Design Basis** 1-AOB max specific growth rate to 0.5 2-NOB substrate NO2 half saturation to 0.1 3-OHO max specific growth rate to 2.5 4-PAO max specific growth rate to 0.1 5-PAO sequestration rate to 2 6a-Anoxic NO2 half saturation switch to 0.01 6b-Anoxic NO2 half saturation switch to 0.1 6c-Anoxic NO2 half saturation switch to 1.0 7a-OHO aerobic yield to 0.67 7b-OHO aerobic yield to 0.72 8a-Particulate substrate COD: VSS ratio to 1.47 8b-Particulate substrate COD: VSS ratio to 1.6 9-Acetate conc to 120

Trial

10a-Alkalinity conc to 500
10b-Alkalinity conc to 1000
11a-DAF capture to 50%
11b-DAF capture to 80%
12-Aeration tanks in series
13a-DO control to 0.5
13b-DO control to 0.7
13c-DO control to 0.3
14a-Air on 6, off 6
14b-Air on 3, off 1
14c-Air on 2, off 2
14d-Air on 1, off 3
15-1.4 Mgal aeration
16-74 Kgal anoxic



QUESTION 4

Why would I want to run lots of simulations with my model?

- a. To understand the results for a range of conditions
- b. To understand the sensitivity of the results to different kinetic rates
- c. To understand the sensitivity of the results to different half saturation constants
- d. To identify capacity limitations
- e. To identify results from diurnal variations
- f. All of the above



PROCESS MODELING

Modeling is beneficial to evaluate current plant performance

Assess various design scenarios to support decisions

However: Garbage in = Garbage out !!!

Important to adequately characterize influent

Which may require a special sampling program

Complex models can also be timely to run

• Thus, design model development should consider the required complexity of the model to evaluate the prospective solution



MODEL OUTPUT

Select model output data and examine output variables during simulation runs

Ensure that simulation proceeds until convergence is reached

Examine model output for consistency with project objectives

Derive required design information



MODELING NOTES AND LIMITATIONS

Simulation packages

- Based on mathematical models
- International cooperation between technical experts
- Default values are averages from hundreds of plants

Site specific wastewater characteristics

- Rigorous sampling programs
- VFA production from primary sludge
- Chemical addition and filtration for P removal.

Resist changing default values

- •Understand differences between model results and full-scale performance first
- Verify with full plant mass balance

Analyze diurnal patterns

Low TN and TP applications

RAMBOLL