Wastewater treatment process modelling

The 5 steps of a modelling project

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INRAE

Aalto University
School of Engineering

Modelling and Control of Water and wastewater treatment processes

WAT - E2130

Outline

- Introduction – Good Modelling Practice (GMP)
- The GMP unified protocol
- Walk through the 5 steps of the unified protocol

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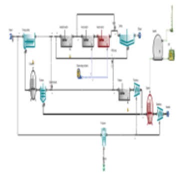
Why a unified protocol?

Wastewater treatment modelling is not trivial!

Process understanding

- Process engineers/technicians
- Different process units compose a WWTP
- Treatment principles: bio-physico-chemical processes take place



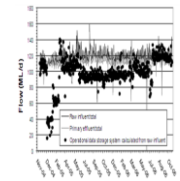
Model understanding

They represent only <u>partially</u> the reality

Simplifications, assumptions need to be understood to interpret simulation results

They required specialised knowledge

They evolve (new variables, new processes…)



Data reconciliation

- Data quality directly affects model quality
- « Garbage in – garbage out »
- Data are always associated with uncertainties

Why a unified protocol?

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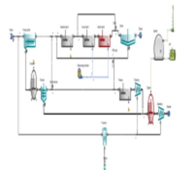
Process understanding

- Process engineers/technicians
- Different process units compose a WWTP
- Treatme
bio-phys
processe



Model ...anding

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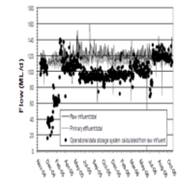
Simplifications

knowledge

They evolve (new variables, new processes…)



Data ...liation

- Data quality directly affects model quality
- « Garbage in – garbage out »
- ...ways
...with
...es

⇨ **To increase quality and efficiency of modelling projects, an internationally accepted protocol was to be developped**

IWA Task Group - Good Modelling Practice

Takayuki Ohtsuki, Japan

Leiv Rieger (chair), Canada

Sylvie Gillot, France

Imre Takács, France

Andy Shaw, United States

Günter Langergraber, Austria

Stefan Winkler, Austria

- Formed in 2005
- Elaboration of Guidelines for Using Activated sludge Models (2012)

Elaboration of a protocol in 5 steps

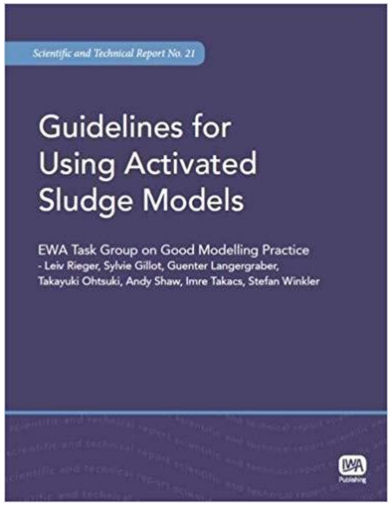
Synthesis of existing procedures

Key steps from protocols related to other domains (hydrology)

14 examples that illustrate the required effort (Application matrix)

IWA Scientific and Technical Report (STR)

Rieger, L., Gillot, S., Langergraber, G., Ohtsuki, T., Shaw, A., Takacs, I., Winkler, S. (2012). Guidelines for Using Activated Sludge Models, IWA Publishing, ISBN: 9781843391746, London, UK, 312 p.



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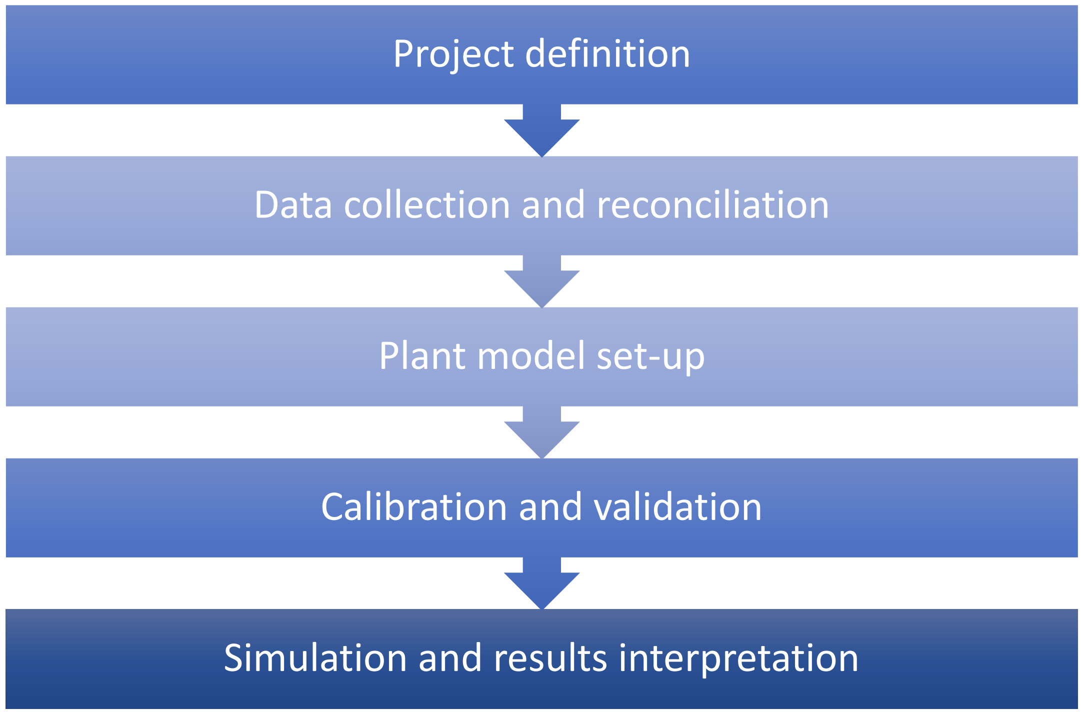
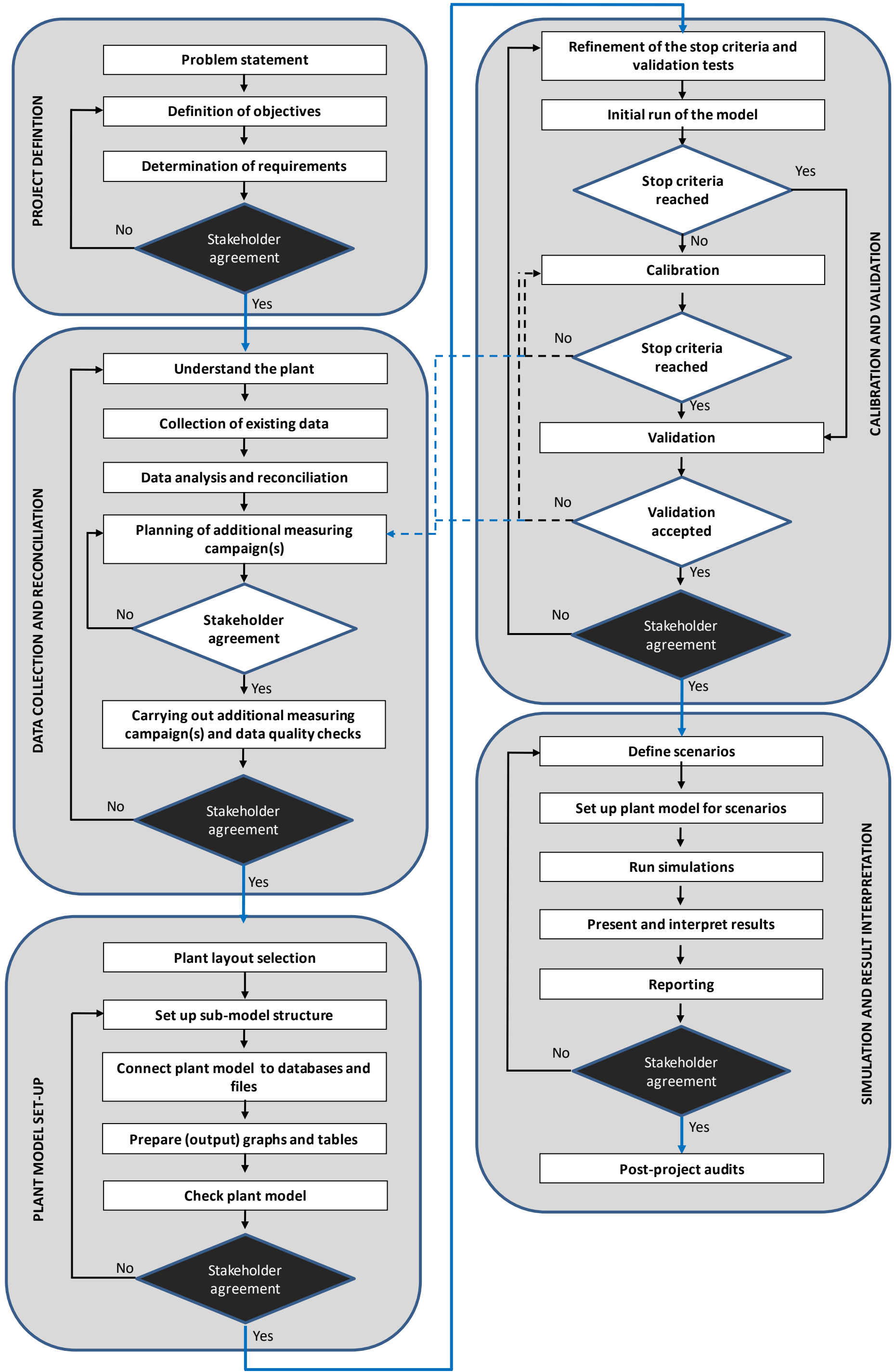
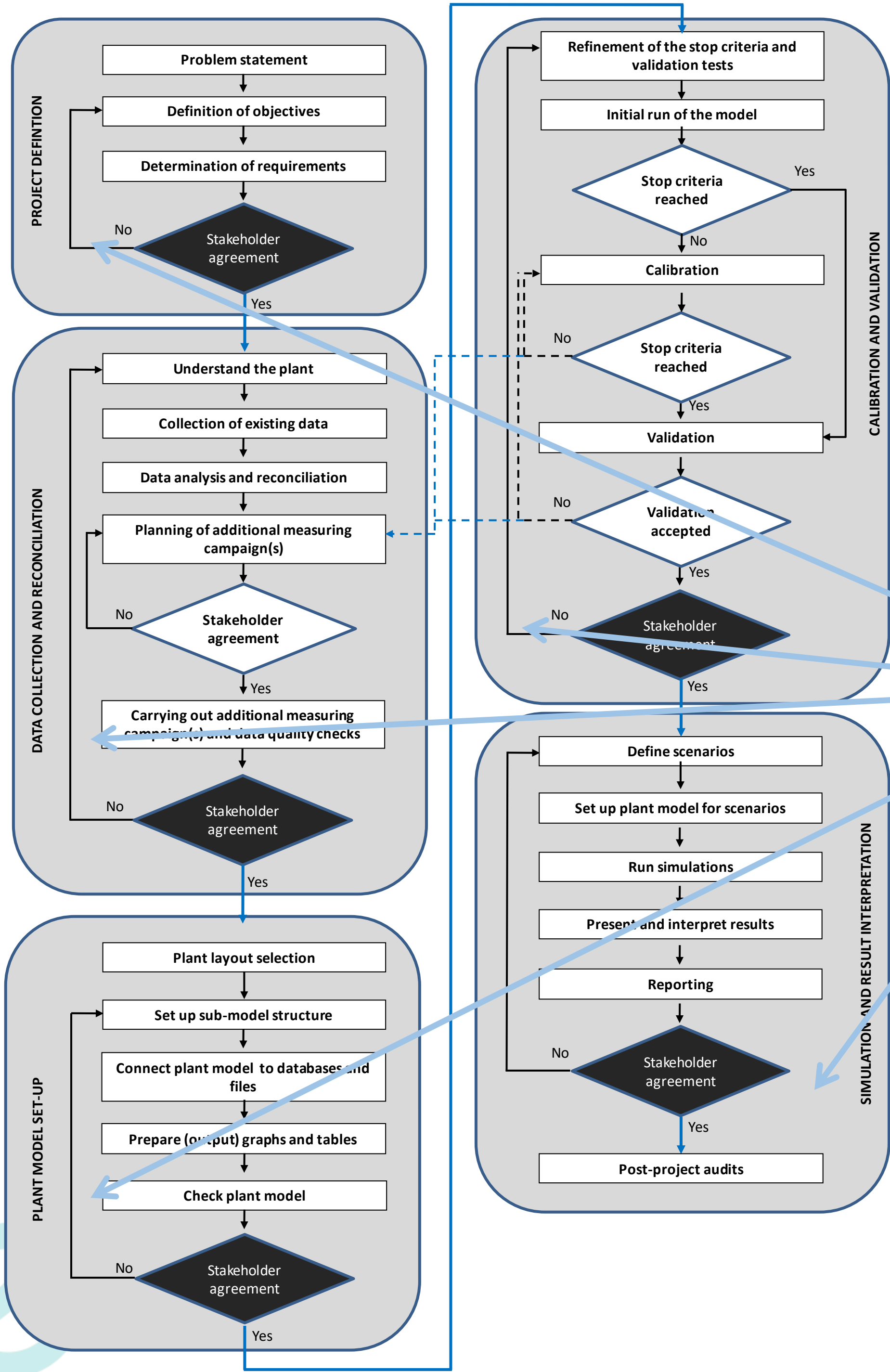
- Walk through the 5 steps of the unified protocol

The GMP Unified Protocol

5 main steps




PROJECT DEFINTION
Problem statement
Definition of objectives
Determination of requirements
Stakeholder agreement
No
Yes
DATA COLLECTION AND RECONCILIATION
Understand the plant
Collection of existing data
Data analysis and reconciliation
Planning of additional measuring campaign(s)
Stakeholder agreement
No
Yes
Carrying out additional measuring campaign(s) and data quality checks
Stakeholder agreement
No
Yes
PLANT MODEL SET-UP
Plant layout selection
Set up sub-model structure
Connect plant model to databases and files
Prepare (output) graphs and tables
Check plant model
Stakeholder agreement
No
Yes
CALIBRATION AND VALIDATION
Refinement of the stop criteria and validation tests
Initial run of the model
Stop criteria reached
Yes
No
Calibration
Stop criteria reached
No
Yes
Validation
Validation accepted
No
Yes
Stakeholder agreement
No
Yes
SIMULATION AND RESULT INTERPRETATION
Define scenarios
Set up plant model for scenarios
Run simulations
Present and interpret results
Reporting
Stakeholder agreement
No
Yes
Post-project audits



Loops until an agreement is reached between modellers and stakeholders

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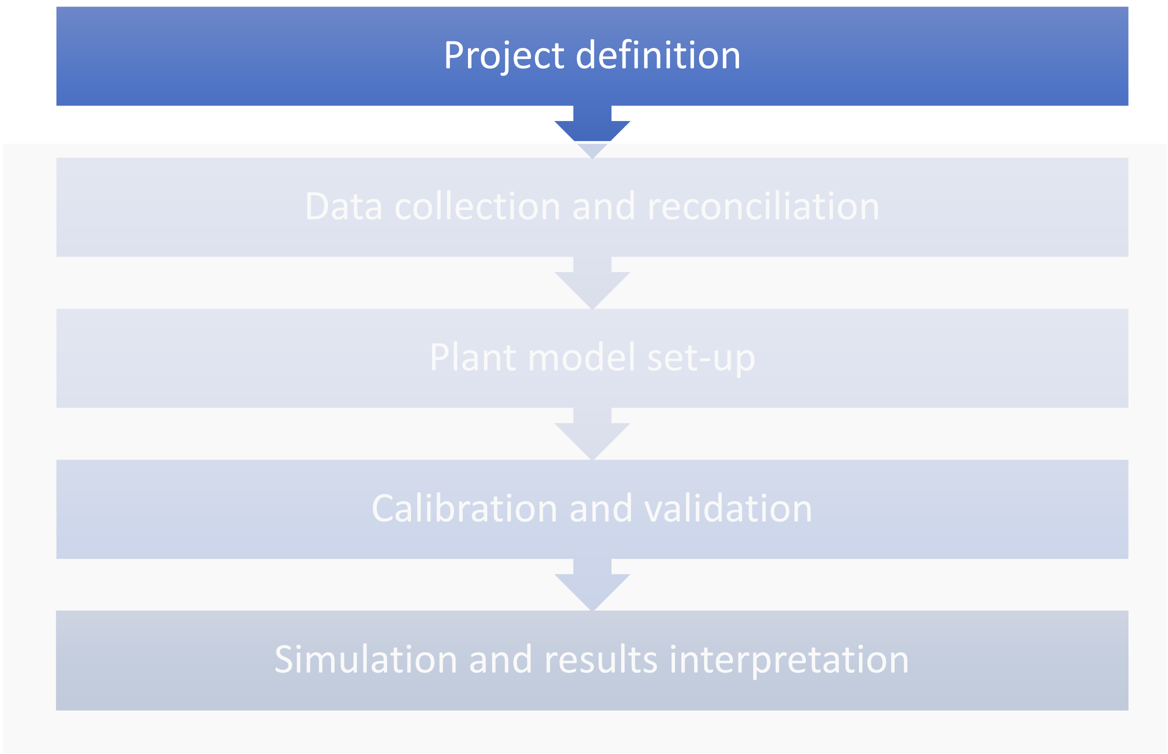
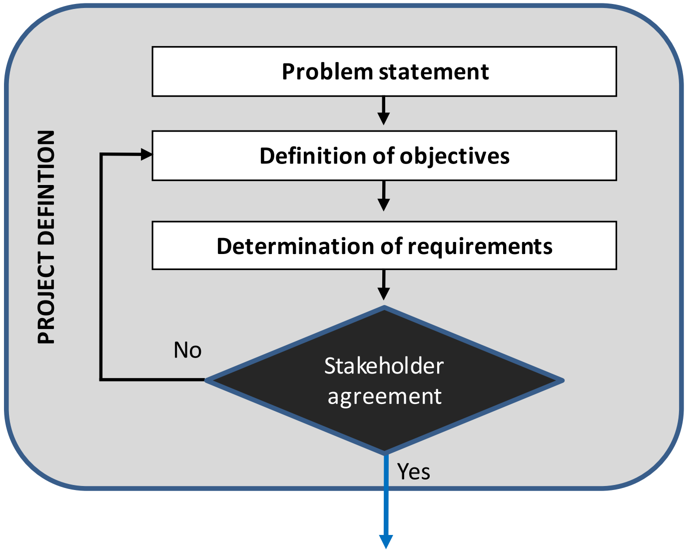


Project definition

Explicit definition of the objectives of the project and of the role of each stakeholder during the project progress

Development of a 'living' document to follow the project: the project definition document



Project definition

Definition of the Objectives

- Boundaries of the model
- Level of complexity (steady state *vs* dynamic)
- Focus variables (calibration, validation) et required accuracy
- Identification of the project stakeholders and their responsibilities
- Constraints (budget, time…)

Requirements

- Personnel (level, experience …)
- Data (quantity, quality)
- Schedule
- Deliverables (reports, models, presentations…)
- Budget

Deliverable

- Project definition document : "dynamic" document that can be altered during the course of the project if agreed by the project stakeholders

Project definition

Examples

Problem statement = Clear and explicit

Aeration system design

≠

Define the peak, average and minimum airflows required for the treatment system under the given design loading conditions

Project definition

Examples

Problem statement

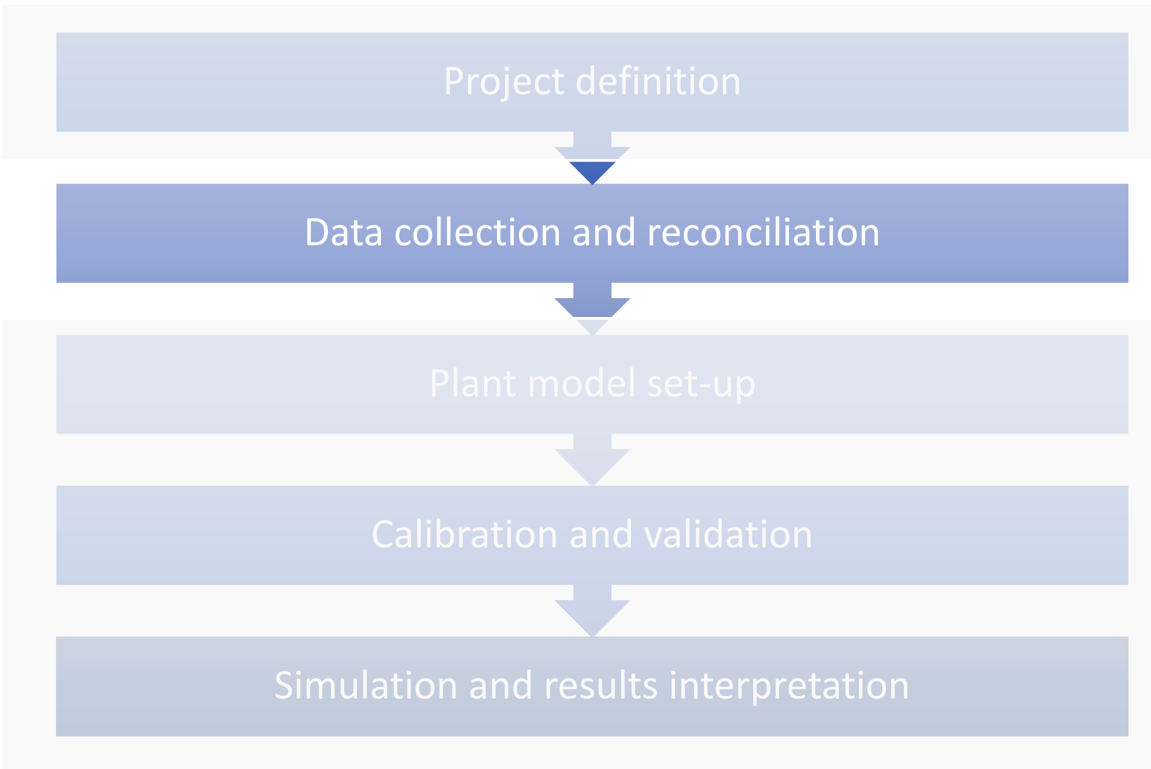
Use the model to assess the plant capacity to treat nitrogen loads

≠

Determine the maximum flow that can be treated under design load conditions to meet required nitrogen removal and effluent limits

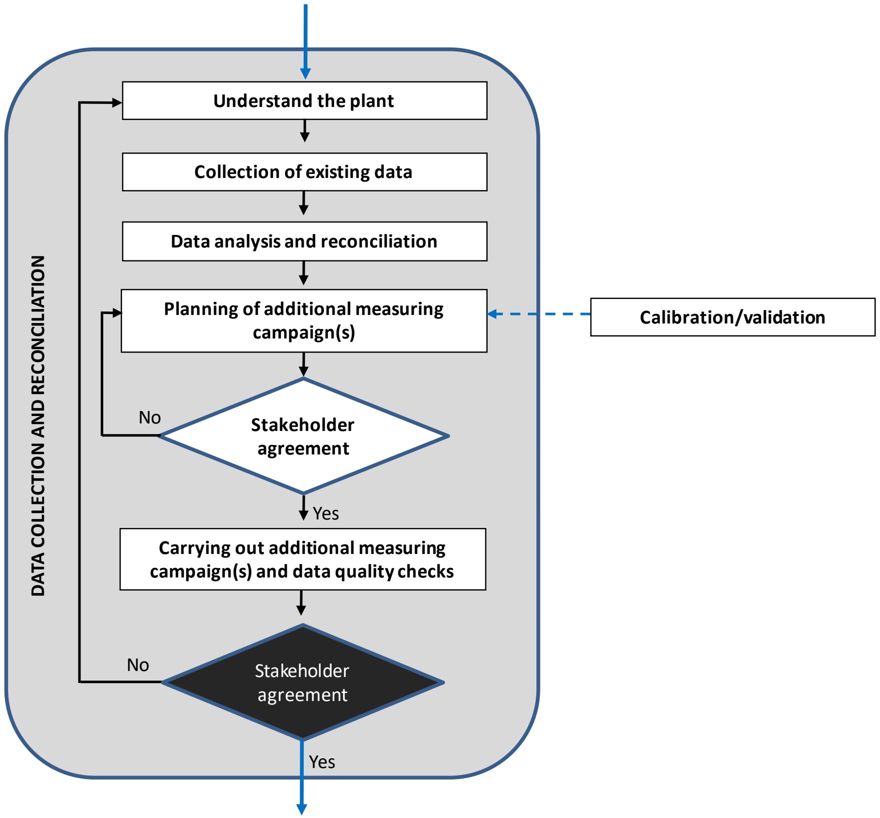
The GMP Unified Protocol

5 main steps



Data collection and reconciliation

More that 1/3 of the required effort in a modelling project

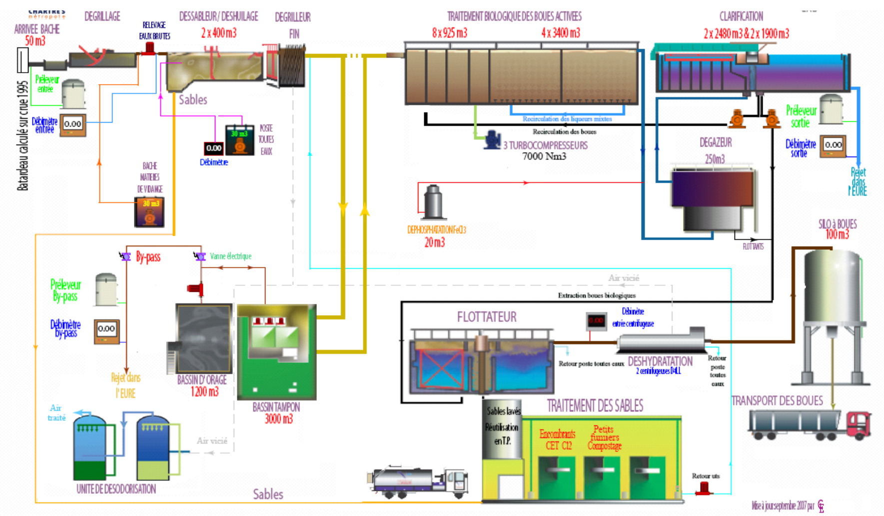


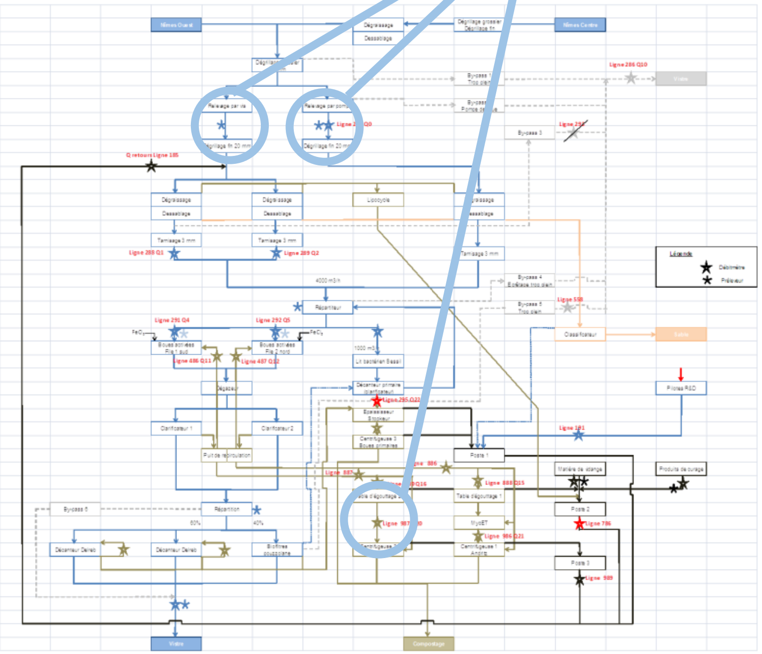
Data collection and reconciliation

Understanding the plant

- Visit the plant
- Update the flow diagram
- Locate sampling points and probes (on line measurements)

Location of flow meters, samplers and sensors





Data collection and reconciliation

Data collection

- Input, output, physical (volumes…), operational (setting points…) data, others
- Historical data: monitoring, operation
- New data: COD fractionation, sampling time, energy…

Data analysis and reconciliation

- Error detection: visualisation, data grouping, comparison with usual data, mass balances
- Reconciliation whenever required

Planning of additional measuring campaign(s)

- Data validation, model calibration and validation (COD fractionation) …
- Stakeholder agreement

Carrying out additional measuring campaign(s)

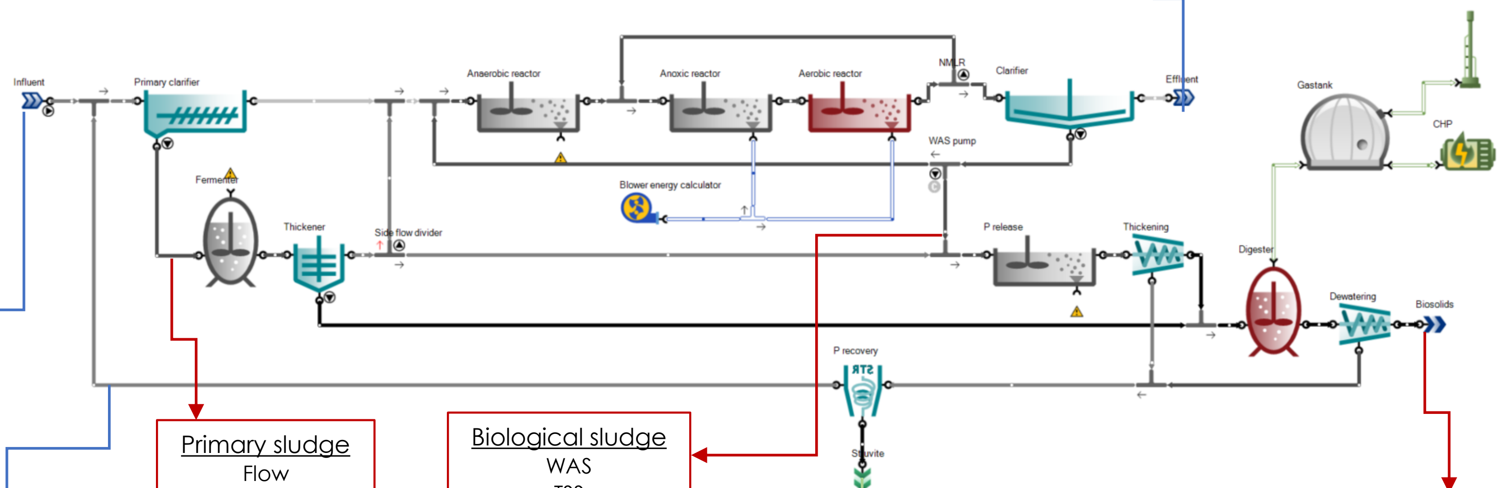
- Data collection

General data requirements

Effluent
Flow
Concentrations
COD
TNK, N-NH_4, N-NO_3, N-NO_2
TSS - VSS
P_{TOT}, P-PO_4
Temperature

Physical data
Tank volumes, surface
Equipments (aeation system, pumps, mixers…)
P&I-diagram
Sludge treatment

Operational settings
DO strategy & set points
Pumping set points
Control strategies
Sludge handlng



Influent/sidestreams
Flow
Concentrations
COD
TNK, N-NH_4, N-NO_3, N-NO_2
TSS - VSS
P_{TOT}, P-PO_4
pH…

Influent fractionation

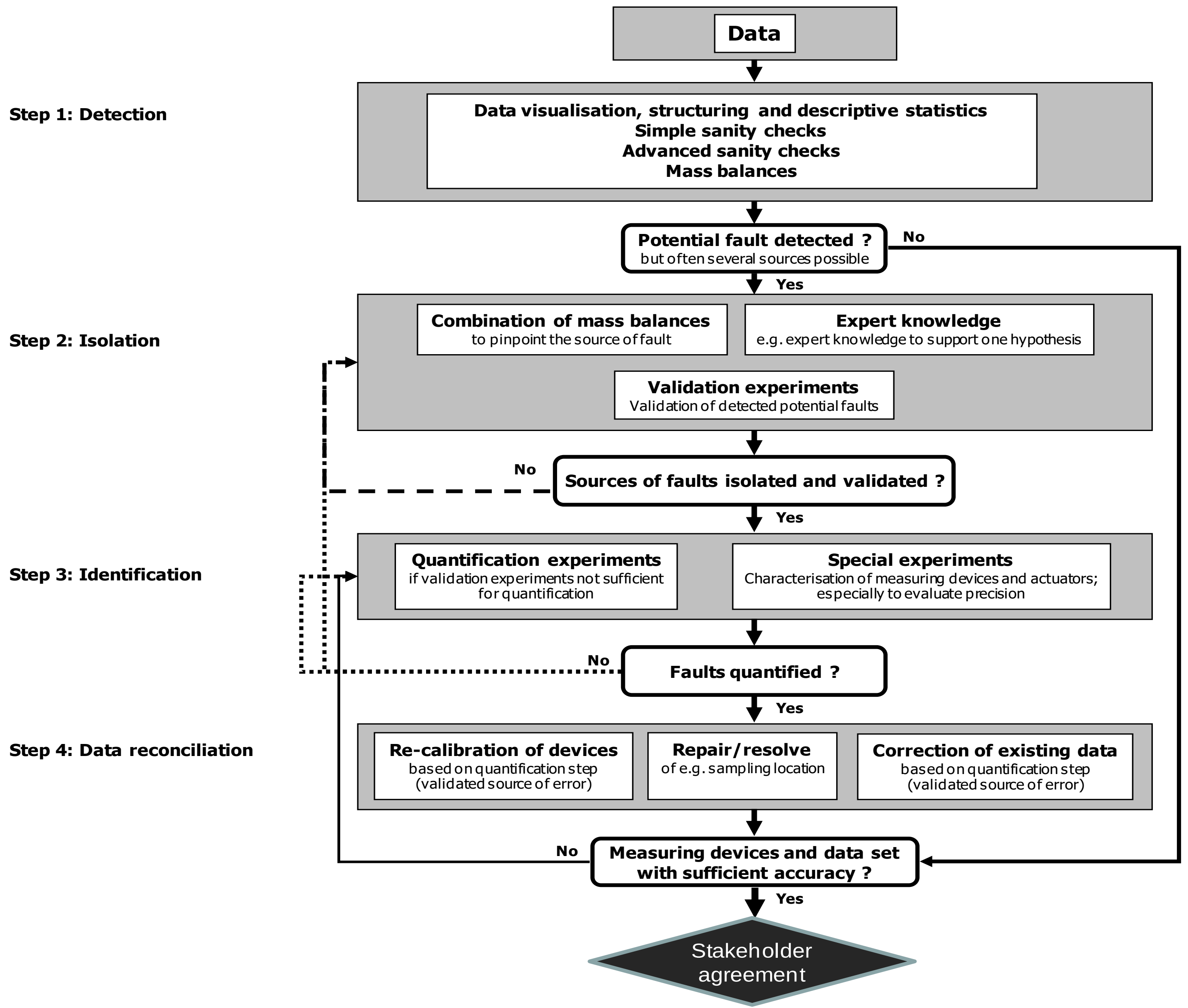
Primary sludge
Flow
TSS
P_{TOT}

Biological sludge
WAS
TSS
P_{TOT}

Nutrient recovery
Mass Flow
Quality

Extracted sludge
Flow
TSS
P_{TOT}

Data analysis and reconciliation

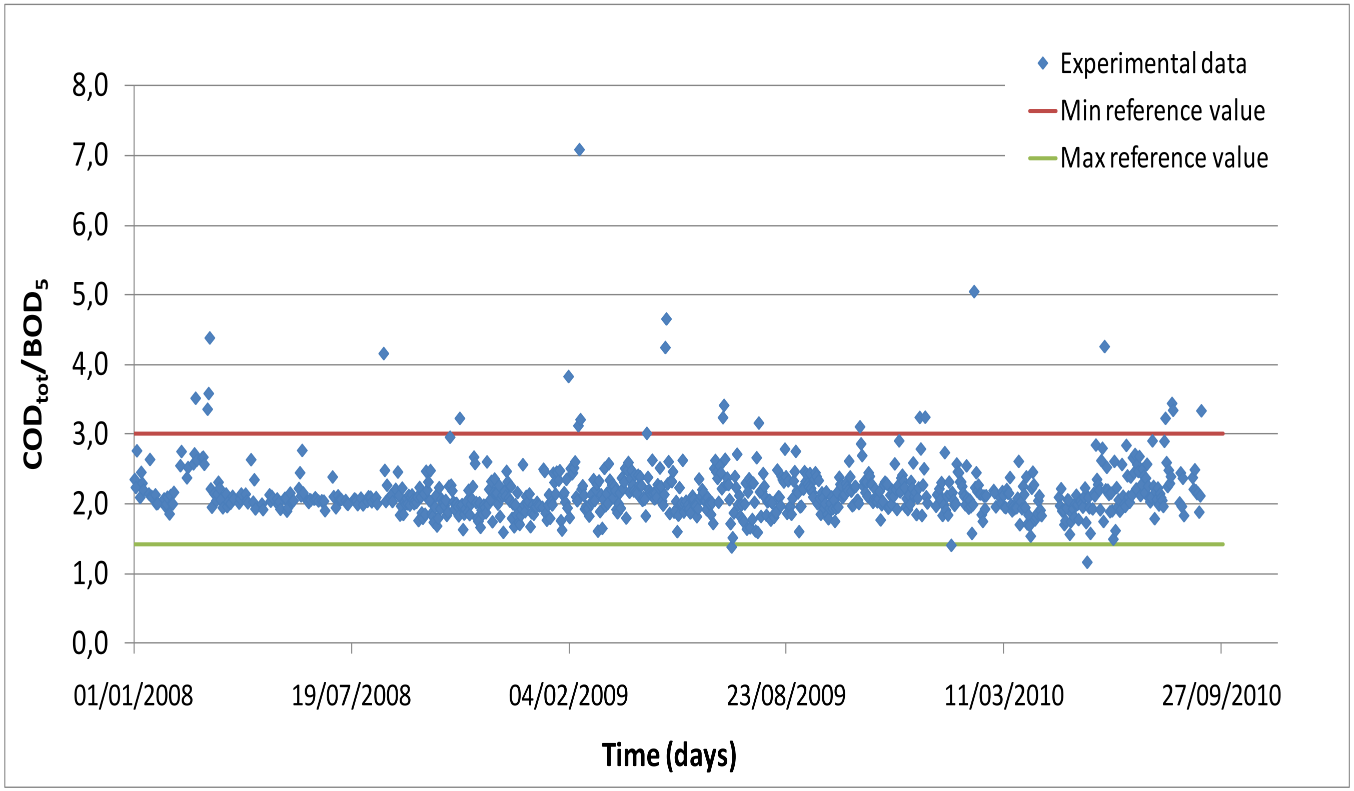


Data collection and reconciliation– Usual Ratios

	Ratio	Unit	n[1)]	**mean**	*Std%* [2)]	**median**	min	max
Raw influent	**N_{tot}/COD_{tot}**	g N/g COD	12	**0.095**	*17%*	**0.091**	0.050	0.150
	$N\text{-}NH_4/TKN$	g N/g N	13	**0.684**	*8%*	**0.670**	0.500	0.900
	P_{tot}/COD_{tot}	g P/g COD	12	**0.016**	*22%*	**0.016**	0.007	0.025
	$P\text{-}PO_4/P_{tot}$	g P/g P	12	**0.603**	*16%*	**0.600**	0.390	0.800
	COD_{tot}/BOD_5	g COD/g BOD	12	**2.060**	*11%*	**2.050**	1.410	3.000
	COD_{fil}/COD_{tot}	g COD/g COD	13	**0.343**	*29%*	**0.350**	0.120	0.750
	TSS/COD_{tot}	g TSS/g COD	12	**0.503**	*18%*	**0.500**	0.350	0.700
	COD_{part}/VSS	g COD/g VSS	11	**1.690**	*12%*	**1.600**	1.300	3.000
	VSS/TSS	g SS/g SS	12	**0.740**	*20%*	**0.800**	0.300	0.900
	BOD_5/BOD_∞	g BOD/g BOD	7	**0.655**	*7%*	**0.650**	0.580	0.740
	Alkalinity	Mol_{eq}/L	11	**5.173**	*35%*	**5.000**	1.500	9.000
Primary effluent	**N_{tot}/COD_{tot}**	g N/g COD	9	**0.134**	*35%*	**0.120**	0.050	0.360
	$N\text{-}NH_4/TKN$	g N/g N	11	**0.755**	*4%*	**0.750**	0.430	0.900
	N_{tot}/COD_{tot}	g P/g COD	9	**0.023**	*25%*	**0.023**	0.010	0.060
	$P\text{-}PO_4/P_{tot}$	g P/g P	10	**0.741**	*12%*	**0.750**	0.500	0.900
	COD_{tot}/BOD_5	g COD/g BOD	9	**1.874**	*31%*	**1.900**	0.500	3.000
	COD_{fil}/COD_{tot}	g COD/g COD	10	**0.449**	*31%*	**0.495**	0.150	0.750
	TSS/COD_{tot}	g TSS/g COD	9	**0.380**	*21%*	**0.400**	0.180	0.560
	COD_{part}/VSS	g COD/g VSS	9	**1.718**	*14%*	**1.700**	1.400	3.500
	VSS/TSS	g SS/g SS	9	**0.794**	*7%*	**0.800**	0.700	0.909
	BOD_5/BOD_∞	g BOD/gBOD	6	**0.644**	*10%*	**0.656**	0.533	0.760
	Alkalinity	Mol_{eq}/L	9	**5.711**	*40%*	**6.000**	1.500	9.000
Activated sludge	**COD_{tot}/VSS**	g COD/g SS	9	**1.434**	*7%*	**1.420**	1.266	1.600
	N_{tot}/COD_{tot}	g N/g COD	7	**0.073**	*35%*	**0.060**	0.045	0.116
	P_{tot}/COD_{tot}	g P/g COD	7	**0.020**	*64%*	**0.015**	0.010	0.044
	VSS/TSS	g SS/g SS	10	**0.739**	*8%*	**0.750**	0.650	0.900

Data collection and reconciliation

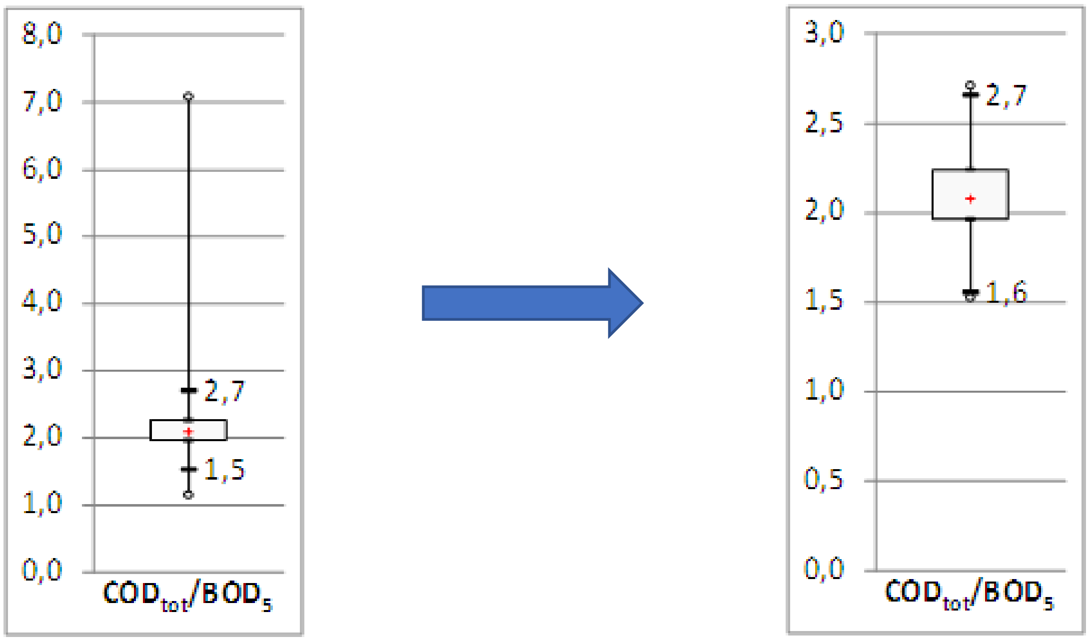
Error detection – usual ratios



Data collection and reconciliation

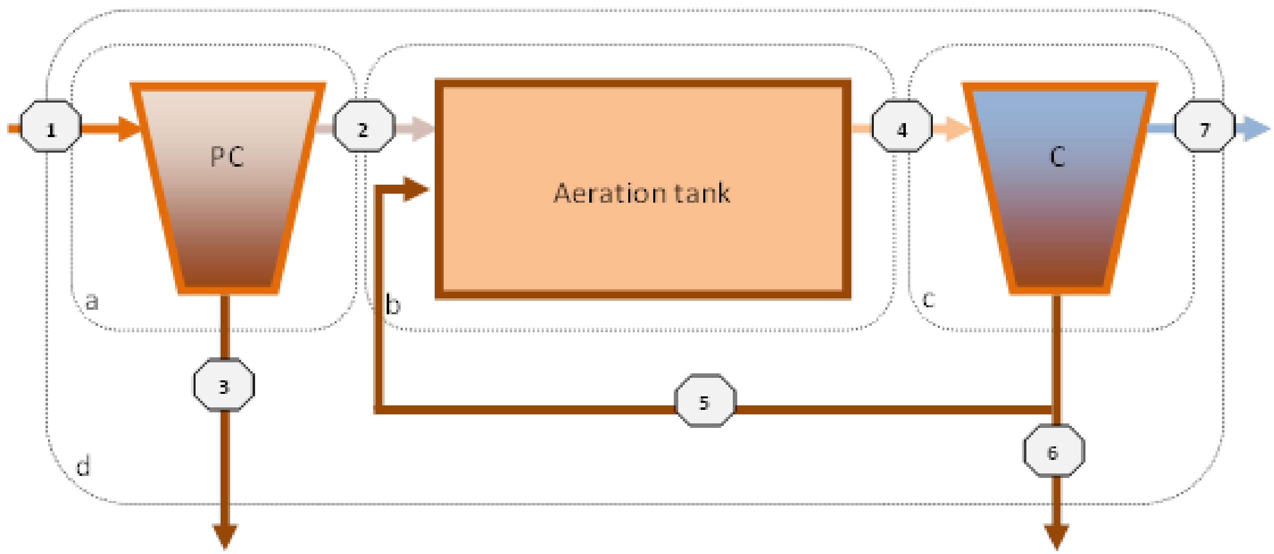
Tukey whisker box

Data analysis



Data collection and reconciliation

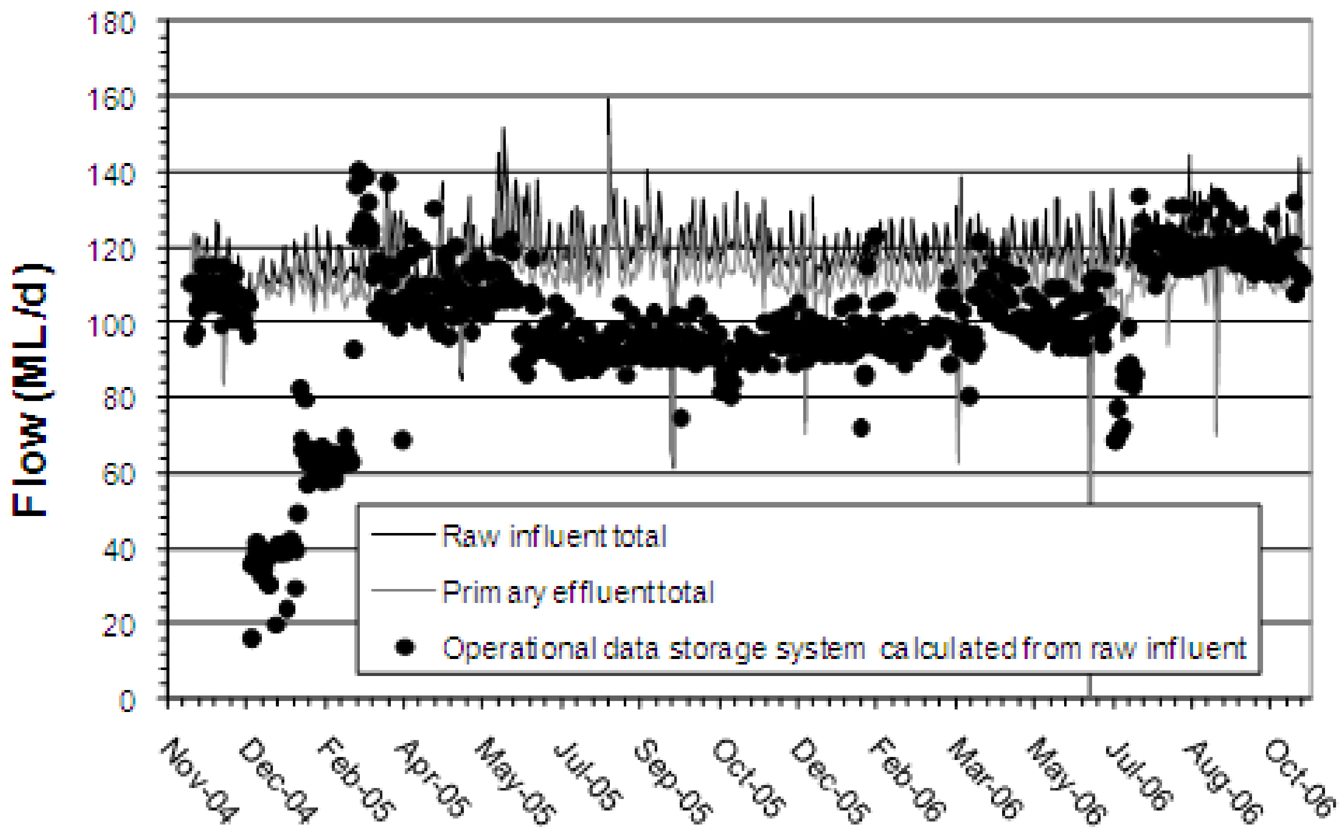
Mass balances



Flux	1	2	3	4	5	6	7
Description	Raw WW	Settled WW	Primary sludge	Bioreactor output	Recycled sludge	Secondary sludge	Effluent

Data analysis and reconciliation

Example 1



Data analysis and reconciliation

Example 2

Usual values		
COD/BOD5	NH4-N/TKN	PO4-P/PTOT
2.4	0.6-0.8	0.6-0.8

	Flow	Concentrations						
Day	m3/j	COD	BOD5	TSS	TKN	NH4-N	PTOT	PO4-P
1	25321	392	163	209				
2	23439	462	190	236				
3	23744							
4	34192							
5	28547	590	214	233	53	37	5.9	4.7
6	28533	383	236	207				
7	34702	499	185	215	50	34	6.1	5.2
8	47566	385	127	193				
9	34960	309	112	165				
10	31971							
11	31790	509	219	253				
12	40982	312	132	173	40	29	5.0	5.0
13	36572	441	223	201	46	46	5.0	5.3
14	47153							
15	41364							
16	37682	264	115	120				
17	32354	329	153	136				
18	33447	530	242	264	51	35	6.2	5.2
19	32940	446	172	213				
20	32753	579	224		54	37	5.9	4.7
21	32097							
22	31383	474	211	201				
23	29897	488	230	222				
24	29441							
25	29965							
26	30526	505	240	210	52	36	5.3	4.1
27	29538	680	215	327				
28	31153	567	23	274	52	34	5.8	5.6
29	30288							
30	29083	440	216	209				
31	28220	452	224	189				

Ratios		
COD/BOD5	NH4-N/TKN	PO4-P/PTOT
2.4		
2.4		
2.8	0.70	0.79
1.6		
2.7	0.69	0.85
3.0		
2.8		
2.3		
2.4	0.72	0.80
2.0	1.00	0.84
2.3		
2.2		
2.2	0.67	0.83
2.6		
2.6	0.67	1.01
2.2		
2.1		
2.1	0.69	0.77
3.2		
24.7	0.66	0.96
2.0		
2.0		

Data analysis and reconciliation

Construct the input datasets

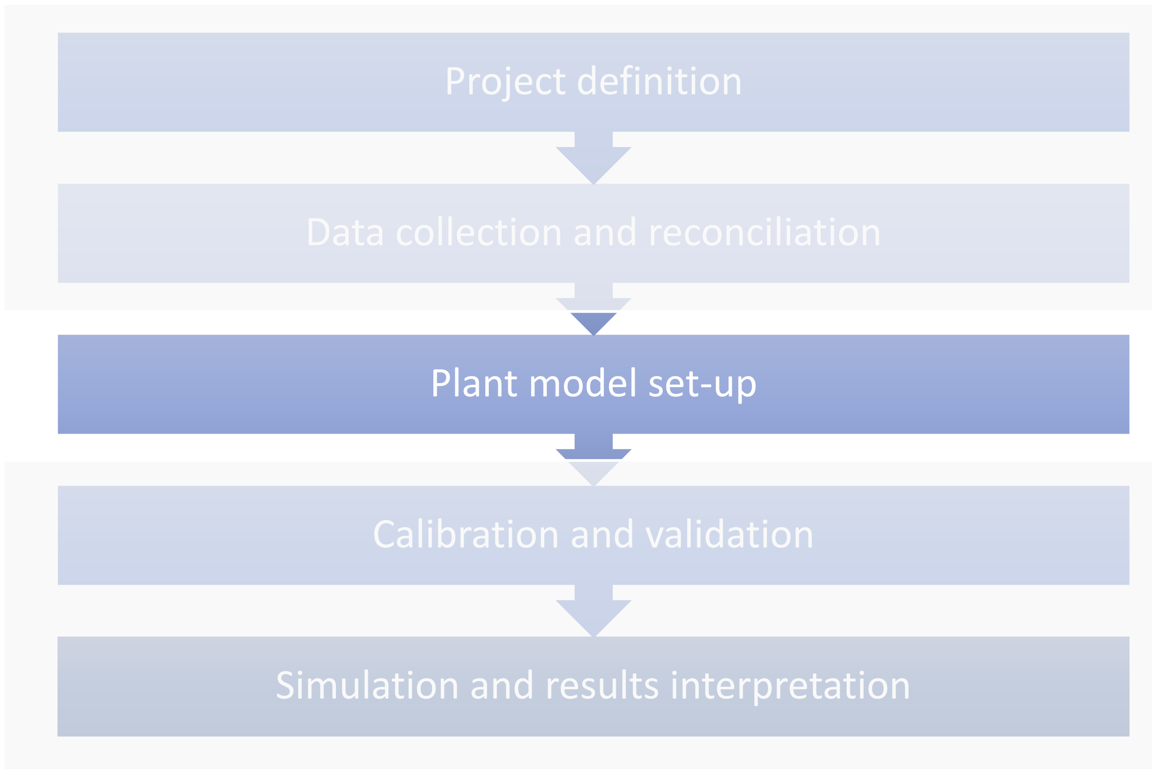
A complete vector of input characteristics

- Missing values should be completed
- Erroneous values should be corrected

    - Data analysis tools more and more used

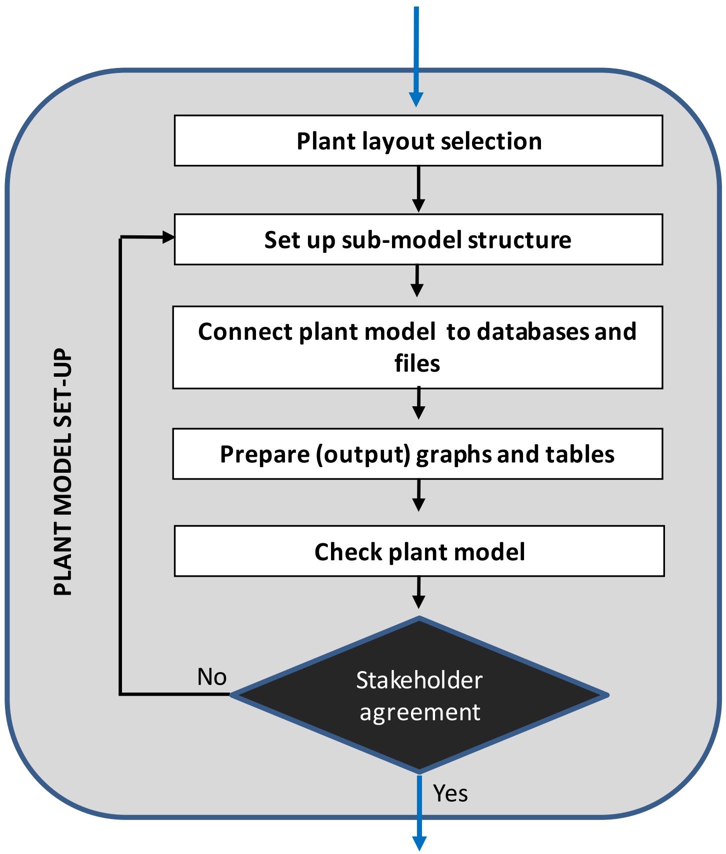
The GMP Unified Protocol

5 main steps

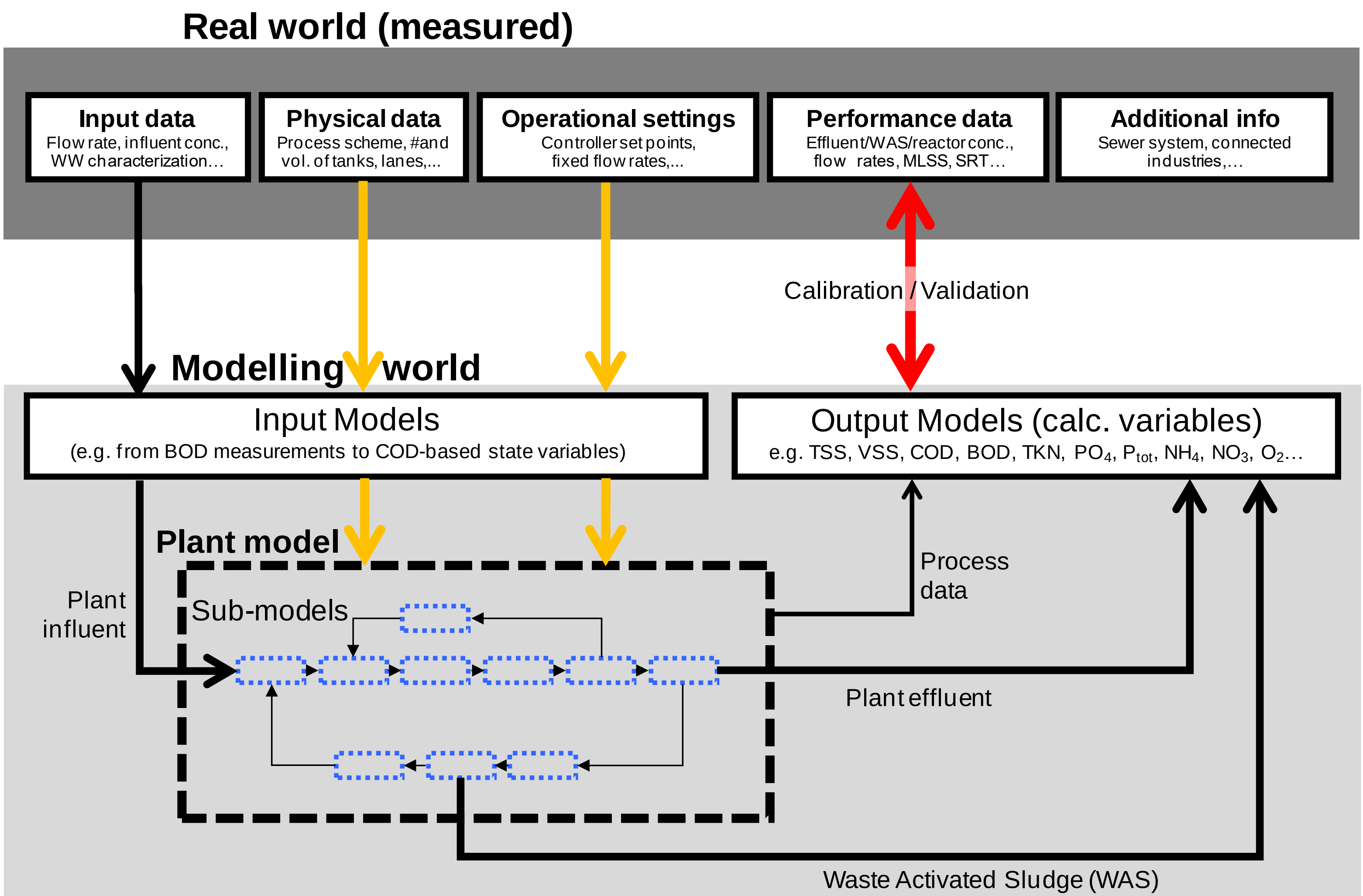


Plant model set-up

Choice of the (number of) reactors and associated models

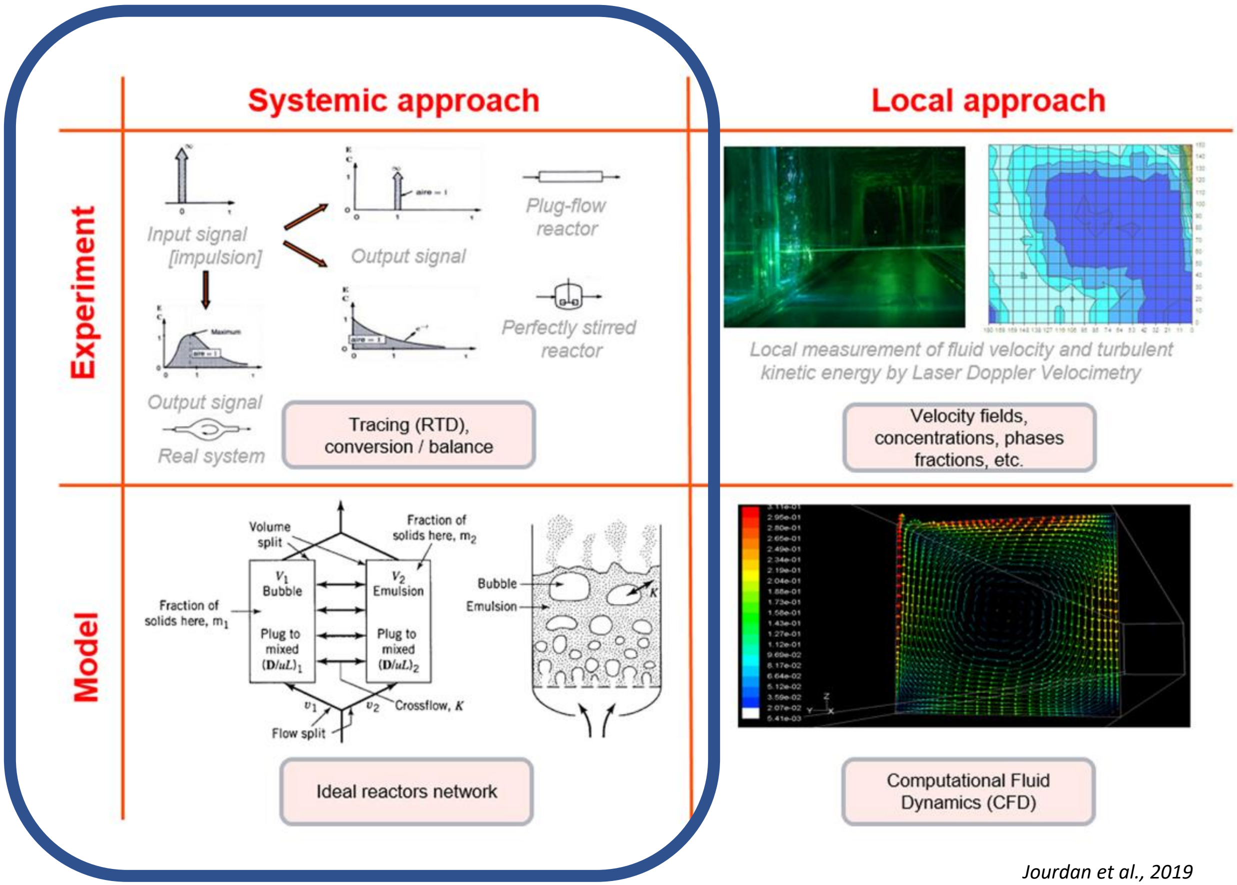


Plant model set-up



Plant model set-up

Mixing behaviour



Jourdan et al., 2019
https://doi.org/10.1016/j.ces.2019.115196

Plant model set-up

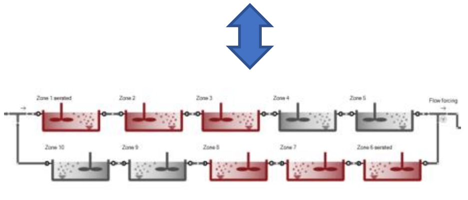
Mixing behaviour

Dispersion is represented by a series of N completely stirred tank reactors (CSTR)

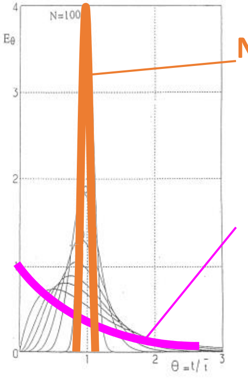
Number and combination of tanks are calibrated on

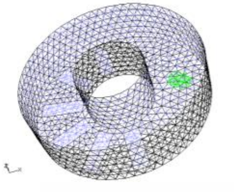
- Experience
- Empirical equations
- Tracer tests
- Computional Fluid dynamics (CFD)

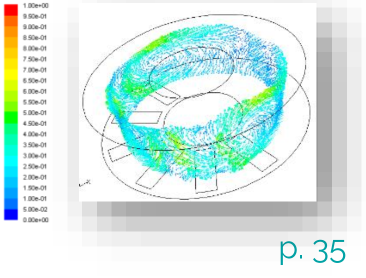
Examples



$$N = \frac{7,4}{WH} LQ_{in}(1+r)$$



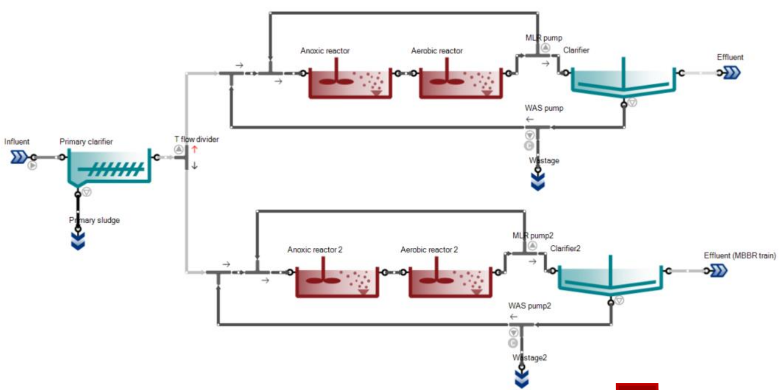


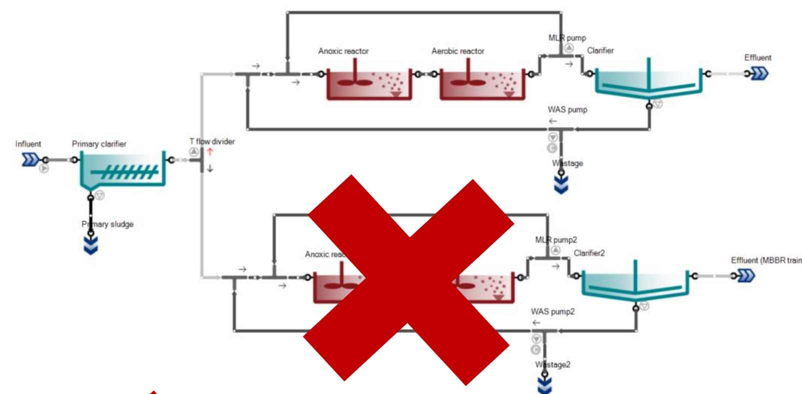


Plant model set-up

- Are all lines operated similarly?
- Which are the main processes?

Low sludge quantity in the clarifier: Point Settler





If TSS1 ≈ TSS2
WAS1 ≈ WAS2
Qrec1 ≈ Qrec2

Plant model set-up

Selection of biokinetic models

"keep it as simple as possible to answer the question"

All processes that significantly affect the target variables

Experience:

- Consulting engineers
- Appropriate defaults parameters available

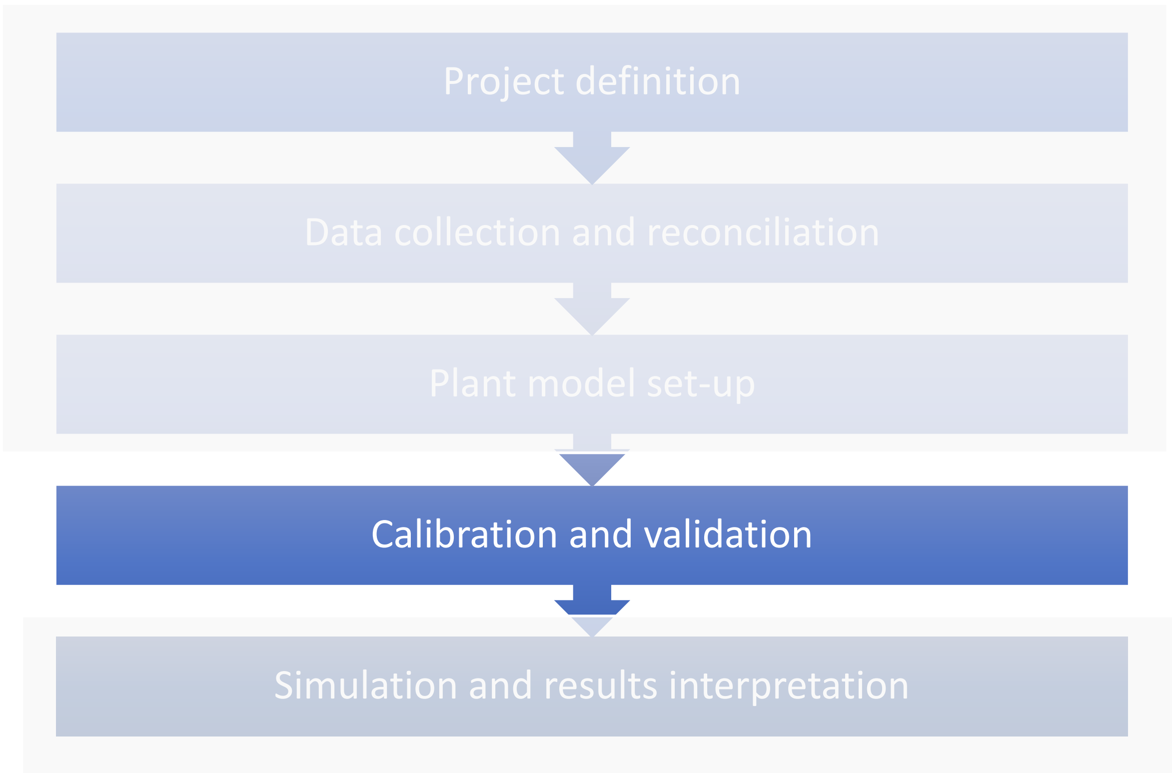
Ease of use

Availability in simulators

Processing time

The GMP Unified Protocol

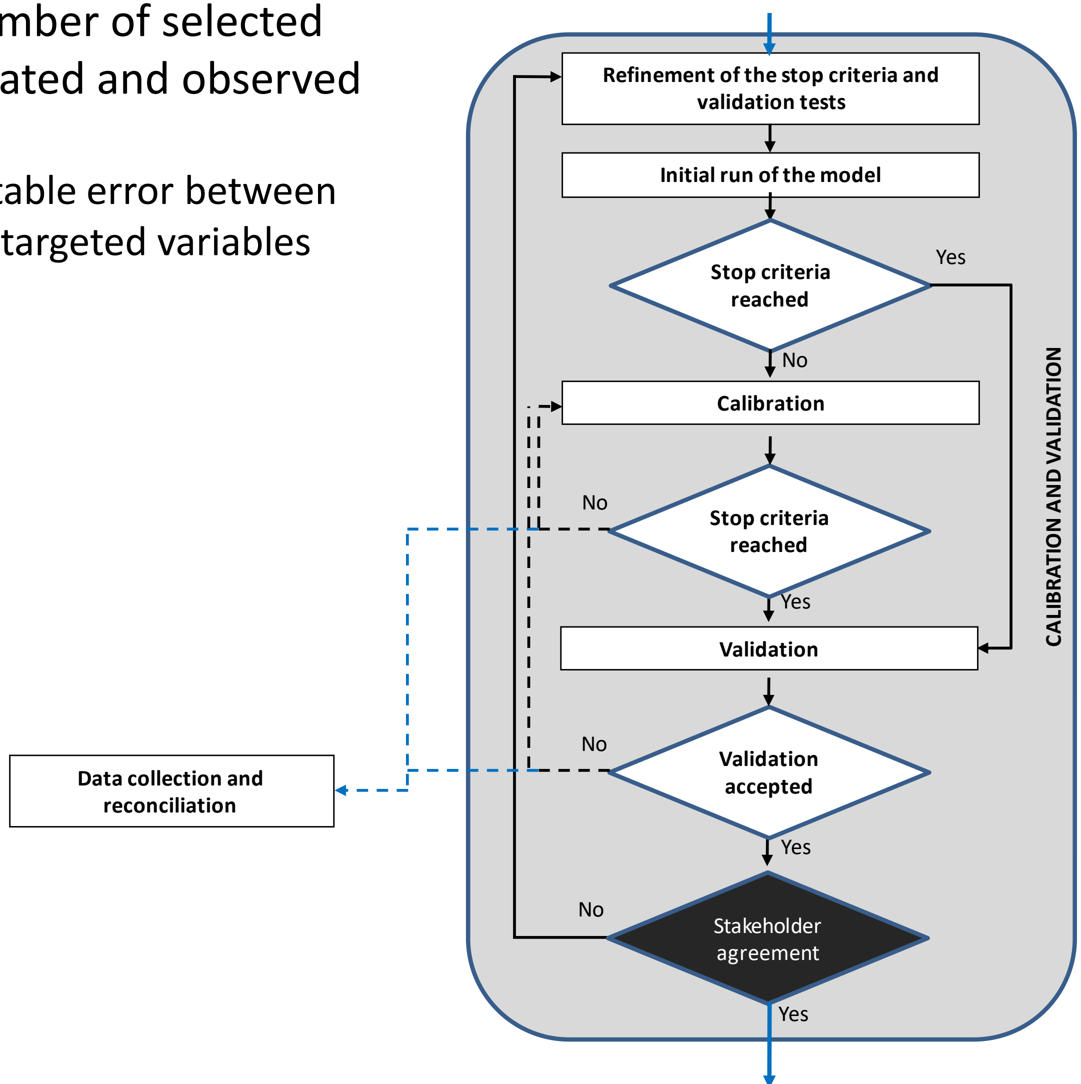
5 main steps



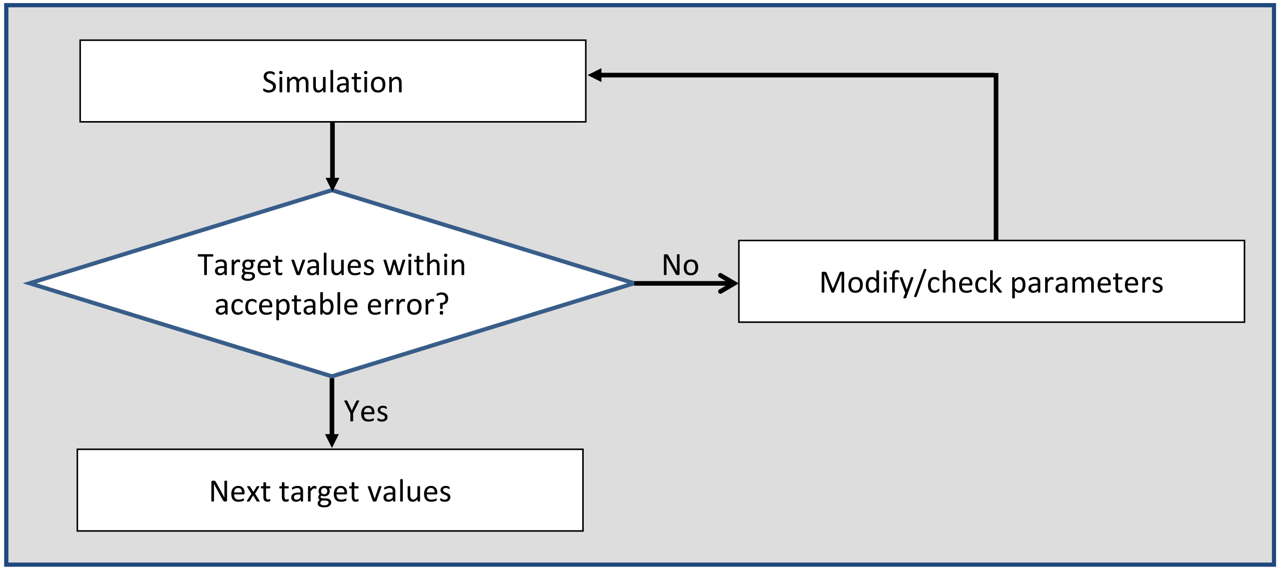
Calibration and validation

Objective : assign the values to a number of selected parameters in order to match simulated and observed data

1. Define a stop criteria => acceptable error between simulated & observed data for targeted variables
2. Select influencing parameters
3. Assign parameter values
4. Validate the parameter set

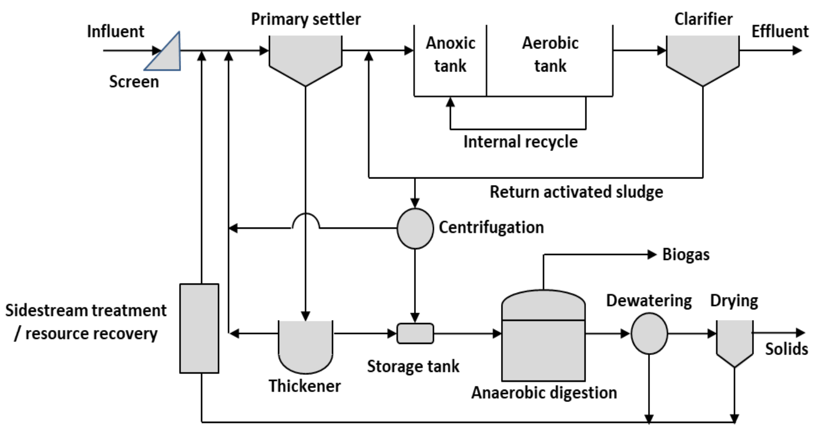


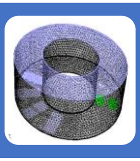
Calibration and validation



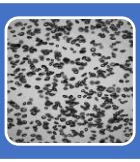
Calibration and validation

Different sub-models required to mimic a plant




Hydrodynamics

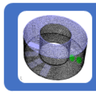
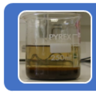
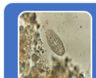

Physico-chemical reactions (precipitation-dissolution, decantation, filtration,...)


Gas - liquid transfer phenomena (aeration, gas emission,...)


Biological reactions (biological conversion of substrates)


Influent characterisation (Organic matter fractionation)

Calibration and validation

-  Hydrodynamics
-  Physico-chemical reactions (precipitation-dissolution, decantation, filtration,...)
-  Gas - liquid transfer phenomena (aeration, gas emission,...)
-  Biological reactions (biological conversion of substrates)
-  Influent characterisation (Organic matter fractionation)

Calibration

How to select influencing parameters?

- Experience
- Published results
- Sensitivity analysis

How to assign values?

- Eyeballing
- Manual fine tuning
- High tech statistical methods
    - Monte carlo analysis
    - …

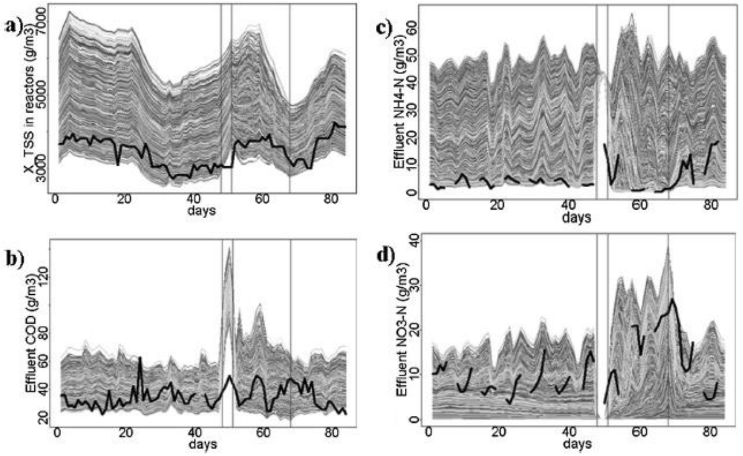


Fig. 1. Results of the n = 5000 simulations for a) Effluent TSS, b) Effluent COD, c) Effluent NH_4–N and d) Effluent NO_3–N. Bold lines correspond to the observed daily composite values. On day 48 all aerators broke down for 3 days, then from day 51 to 68 the aerators were running permanently (days 48, 51 and 68 indicated by vertical lines).

Hauduc et al., 2015
https://doi.org/10.1016/j.envsoft.2015.02.004

Calibration

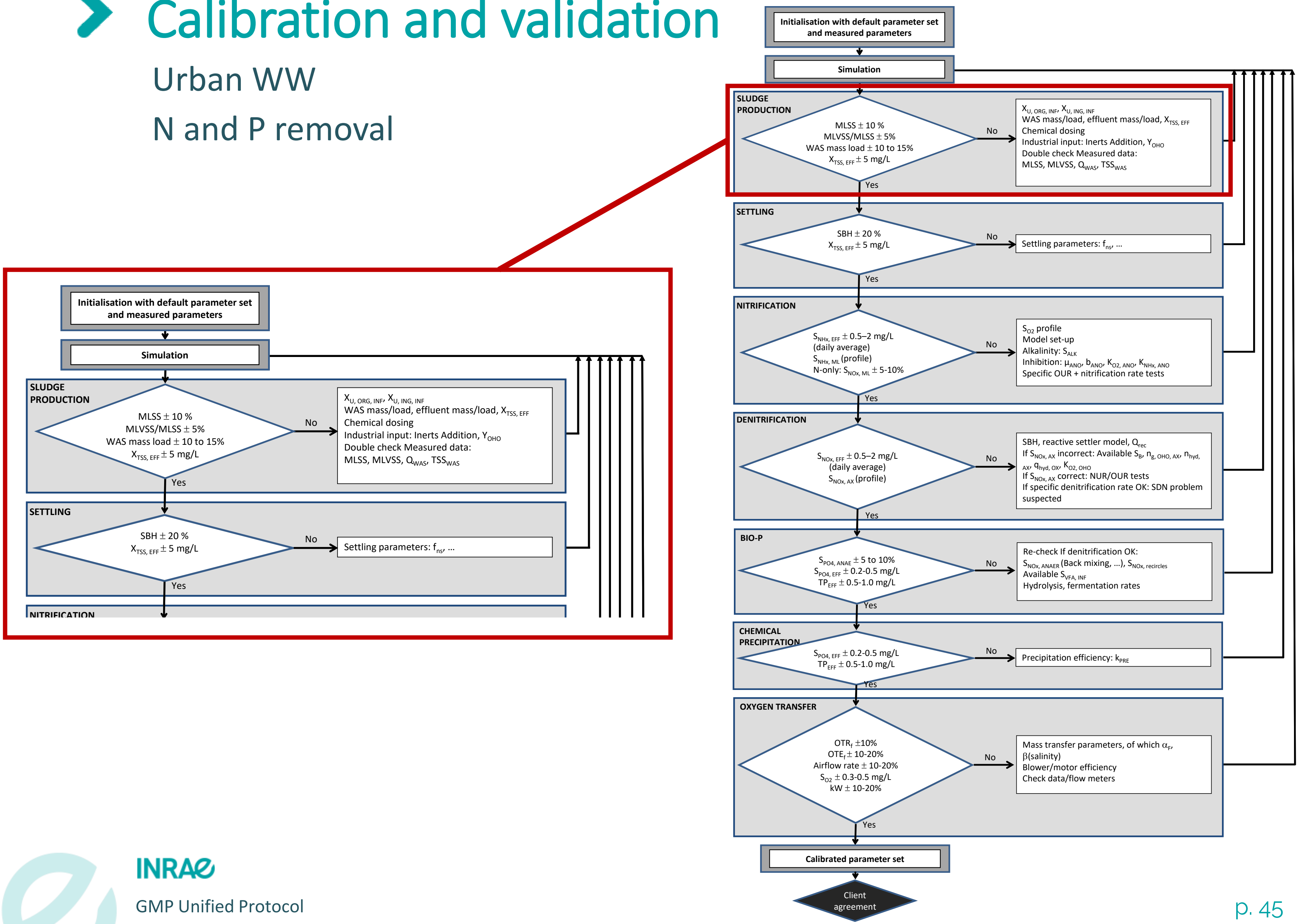
- Keep in mind
  - WWT process models have a low identifiability
  - Data quantity and quality have a huge impact
  - Default parameter sets exist for urban WW, they may be different:
    - for industrial WW
    - for new processes…
  - An order to follow:

1. Structure/hydrodynamics
2. Influent characterisation
3. Biocinetic parameters

Calibration and validation

Urban WW

N and P removal



Validation

A subject under debate!

Validation = is the model fitting for the purpose, i.e. able to:

- describe observed behaviour
- support engineering decision

Objective = to define the domain of validity of the model

Engineering experience may be used to check results

Usually, a different dataset is used for calibration and validation: different operating conditions, flows, temperature…

The GMP Unified Protocol

5 main steps

Project definition

↓

Data collection and reconciliation

↓

Plant model set-up

↓

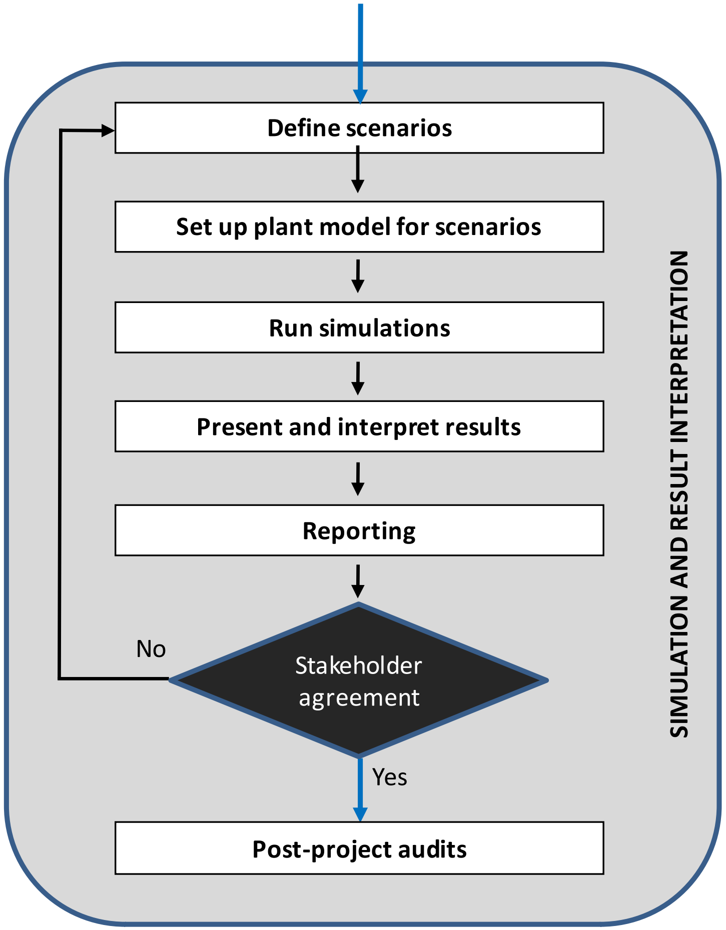
Calibration and validation

↓

Simulation and results interpretation

Simulations et results interpretation

Different scenarios



Simulations et results interpretation

Definition of the scenarios

- Steady state, dynamic

Model

- Modifications, input data

Simulation

- For the different scenarios, steady state vs dynamics

Presentation et results interpretation

- Graphs, tables…

Reports

Simulations et results interpretation

What if scenarios

What if the plant experiences a storm flow?

What if we change the operating schedule for sludge dewatering?

What if a tank is taken offline?

What if an industry closes and it no longer discharges to the plant?

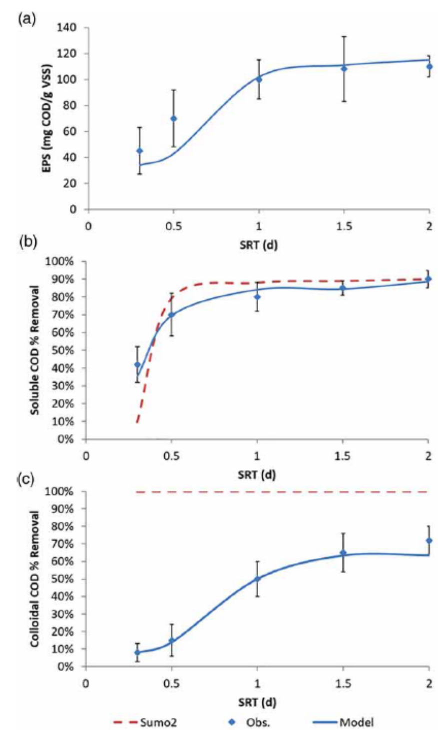
WHAT IF…??

Sensitivity analysis

What is the impact of the sludge age, the recirculation ratio, DO levels…

Steady state or dynamic simulations?

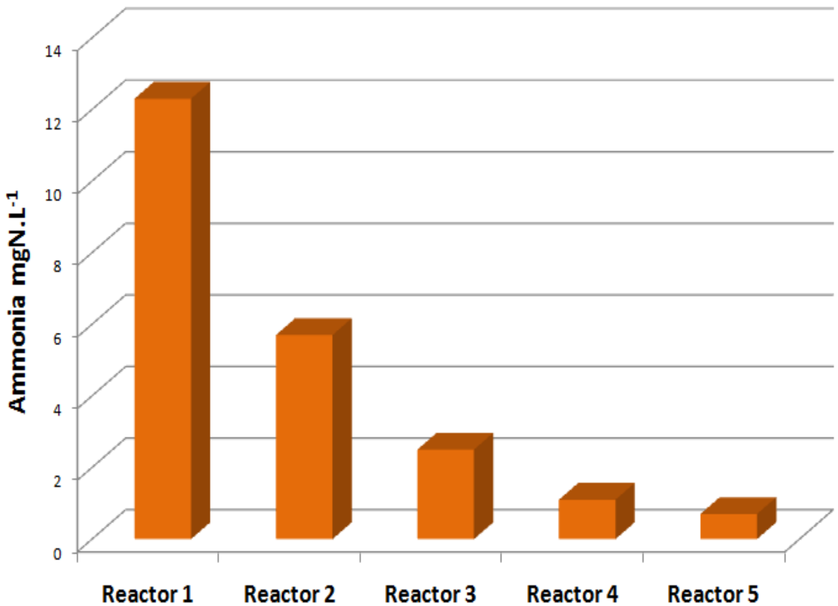
Steady state	Dynamic
Long-term performance	Short-term performance
Less data intensive	More data
Overall issues	Detailed investigations
Quicker	More time



Hauduc et al., 2019
https://doi.org/10.2166/wst.2018.454

Simulations et results interpretation

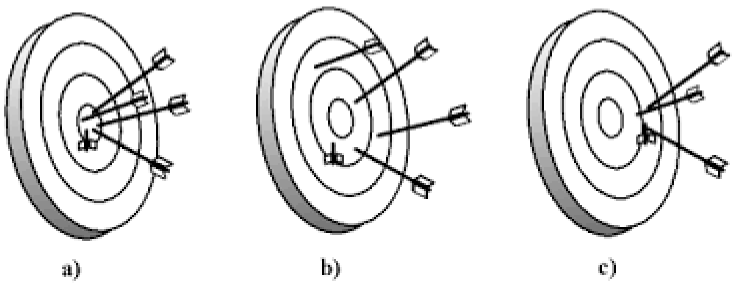
Simple example – Results presentation



Steady State Simulations	Dynamic Simulations
Tables	Graph of time-based outputs
Bar Graphs, Line Graphs and Pie Charts	Animated versions of Bar Graphs, Line Graphs and Pie Charts
Process Flow Diagram	Table of Output Data and Summary Statistics

Closing remarks

Data may be wrong too!



Be a process engineer first!

Be aware of the limitations / the domain of validity of your model

Wastewater treatment process modelling

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