/innovation

Plant wide chemical water stability modelling with PHREEQC for drinking water treatment

Alex van der Helm	Waternet / Delft University of Technology
Onno Kramer	Waternet
Jos Hooft	Waternet
Peter de Moel	Omnisys/ Delft University of Technology

2nd IWA New Developments in IT & Water Conference, Amsterdam, the Netherlands, February 10th 2015

/innovation

Waternet

Water cycle company of Amsterdam:

- Drinking water production and distribution
- Waste water collection and treatment
- Water system management
- Water safety (dikes)
- Nautical and waterway control

/innovation

Calculating in PHREEQC

pH – **Re**dox – **Eq**uilibrium – **C**alculations

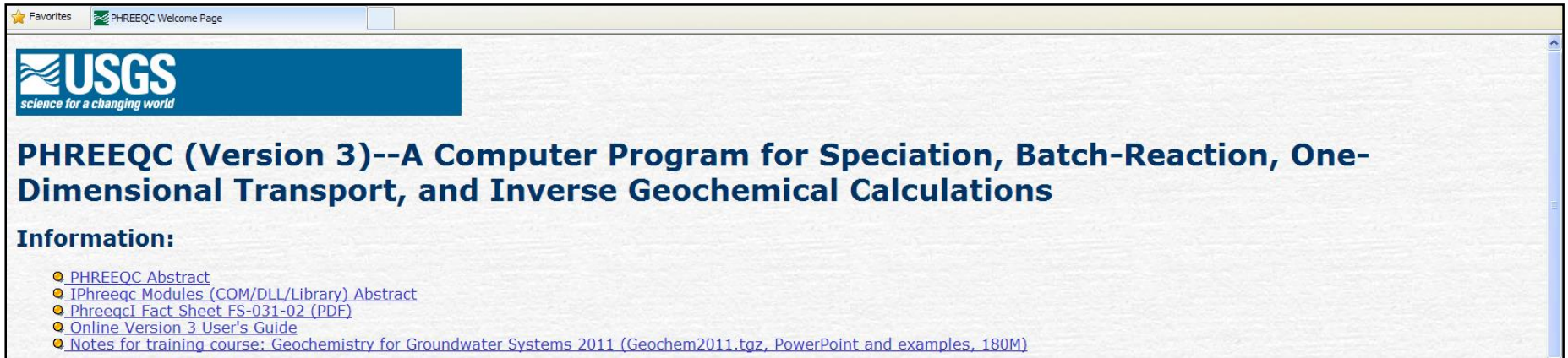
- developed by US Geological Survey (USGS)
- scientific base, fully traceable
- adapted to newest scientific knowledge
- users can modify and extend the basics
- communication with MS Excel possible
- freely available

/innovation

Calculating in PHREEQC

pH – **Re**dox – **Eq**uilibrium – **C**alculations

- 25 elements
- Liquid, gas and solid phase
- 8 databases with equilibrium constants



/innovation

Stimela.dat

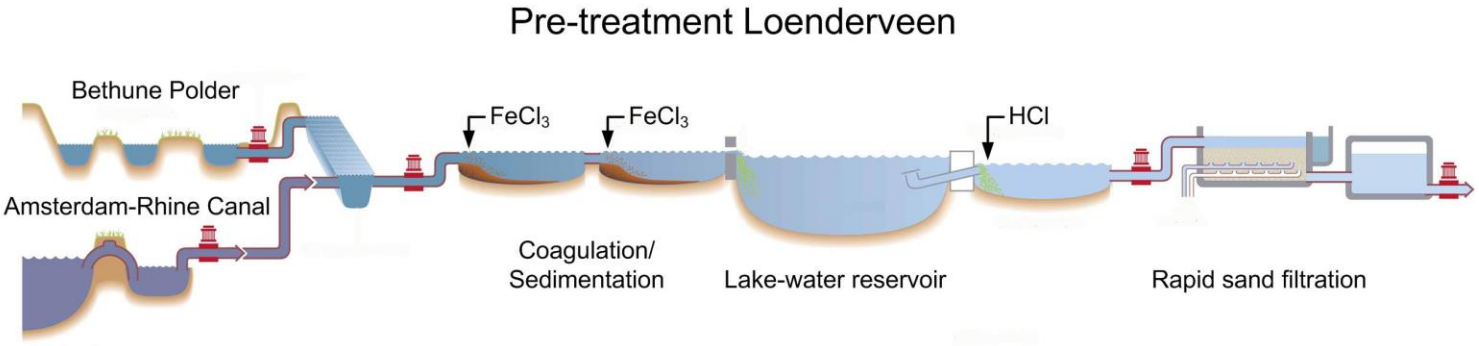
De Moel et al. (2014) developed PHREEQC database **Stimela.dat** for water treatment

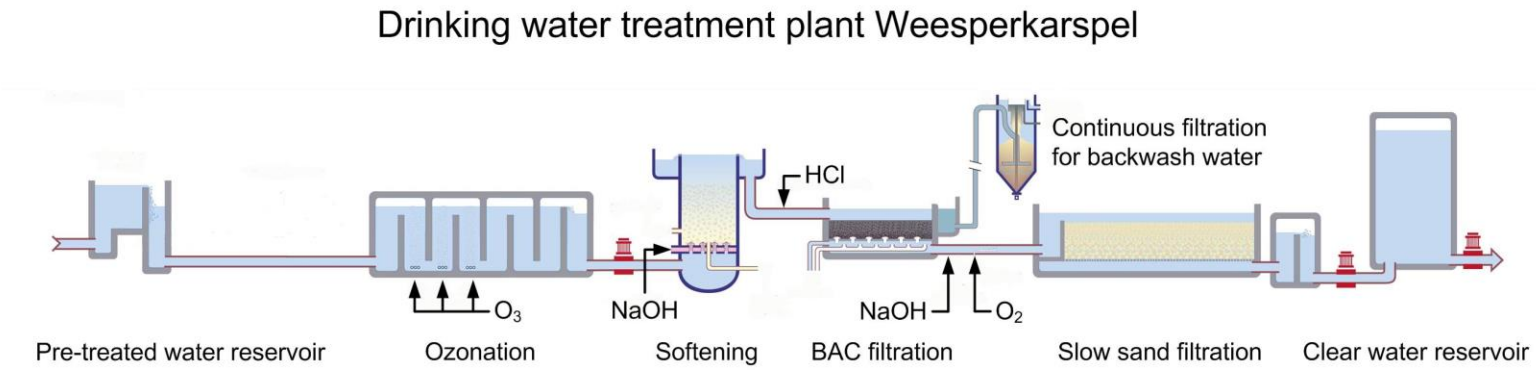
Inert elements were defined for:

- Oxidation states of nitrogen NH_4^+, N_2, NO_2^-
- Anaerobic groundwater species Fe^{2+}, Mn^{2+}
- Anaerobic gases CH_4, H_2S, NH_3

/innovation

Drinking water treatment plant

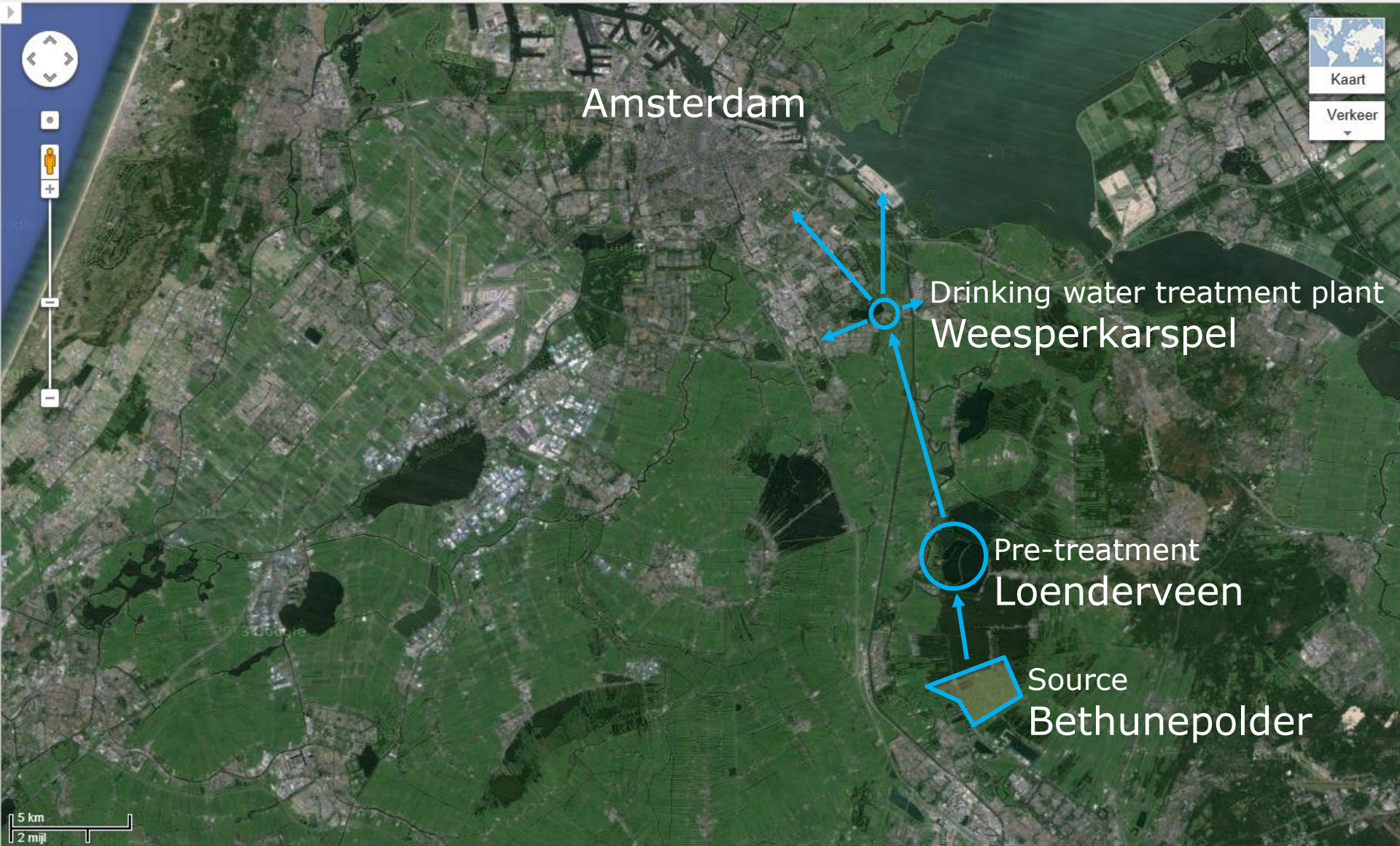




waternet

/innovation

Loenderveen-Weesperkarspel



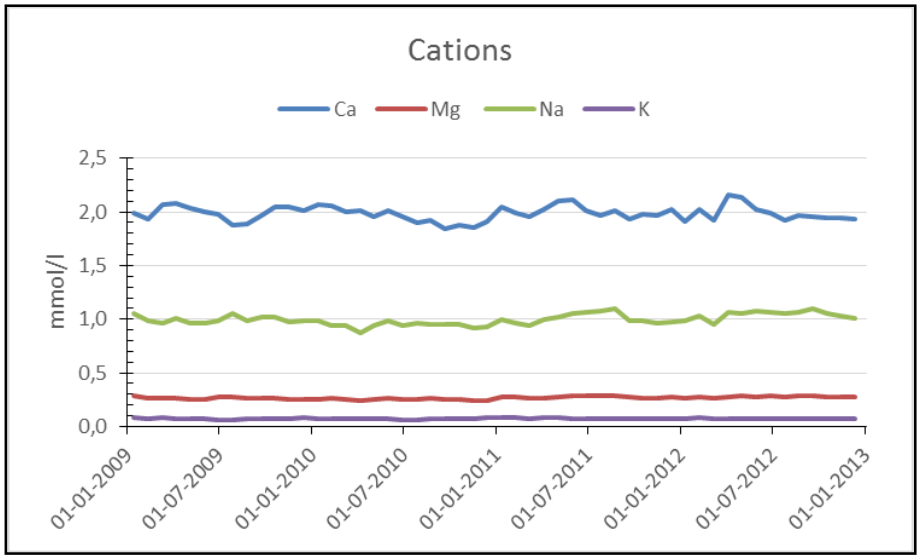
/innovation

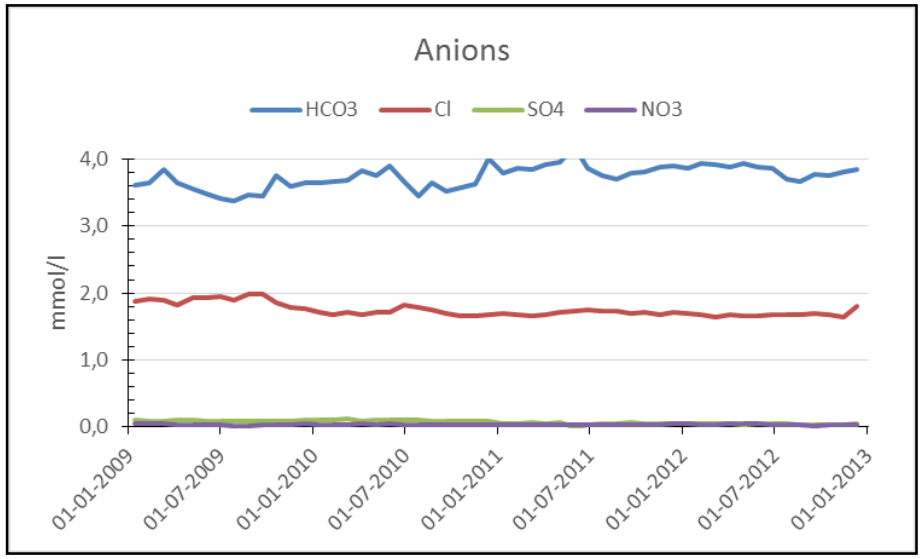
Lake water reservoir

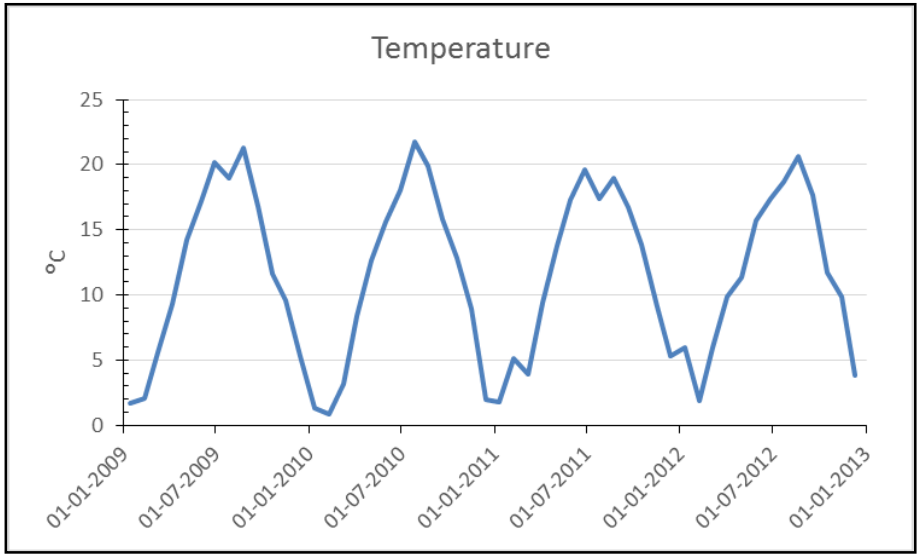
waterunet

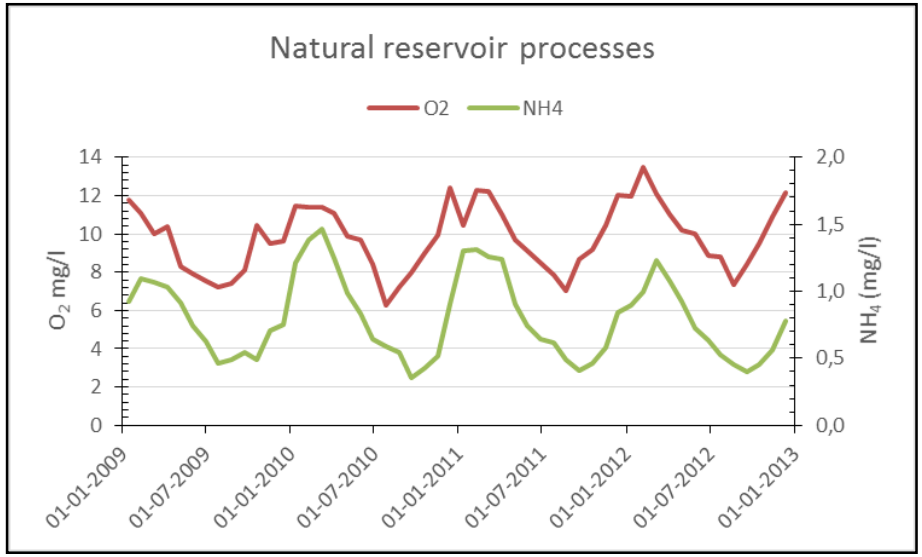
/innovation

“Raw water” parameters



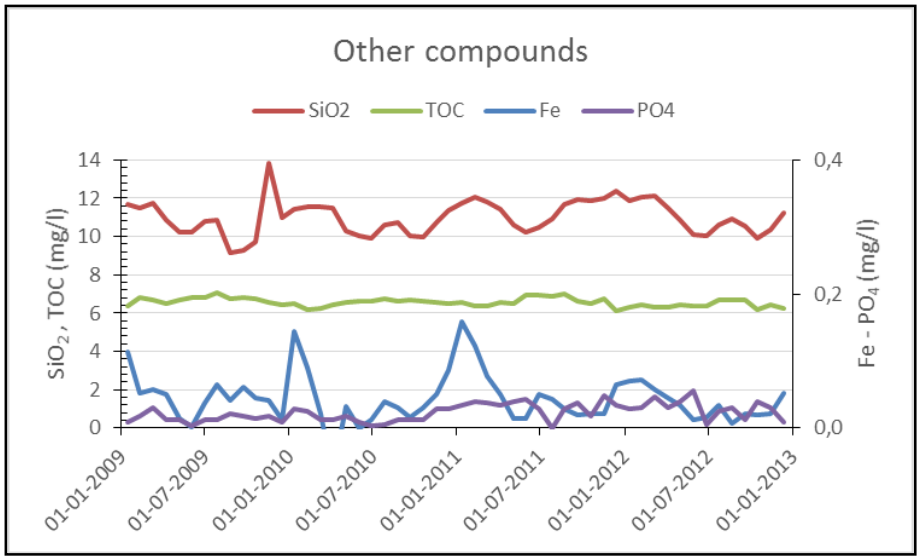


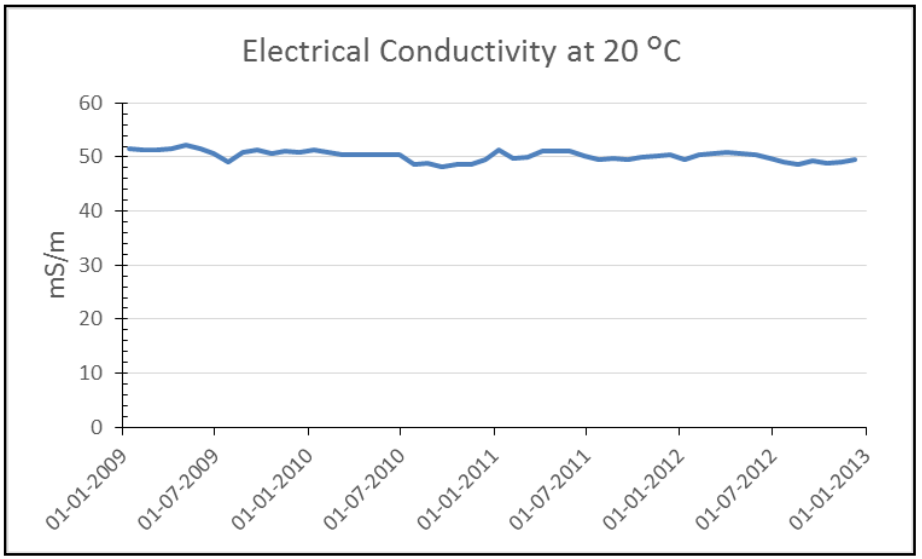




/innovation

Raw water parameters

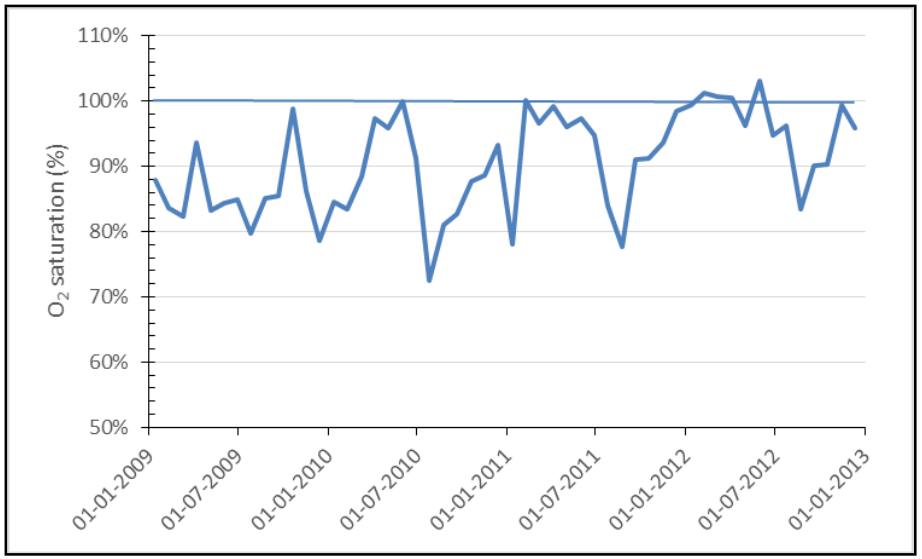




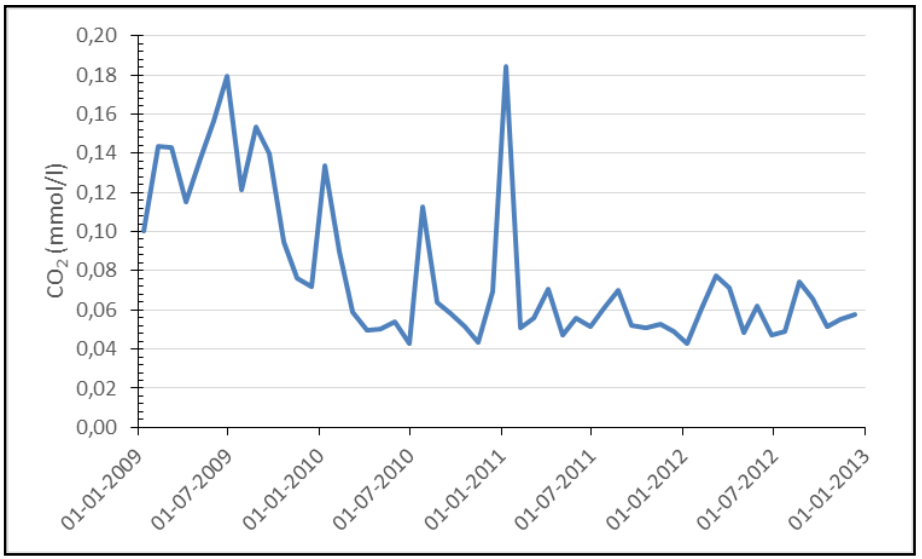
waternet

/innovation

Raw water evaluation with Stimela.dat



Calculated Oxygen saturation

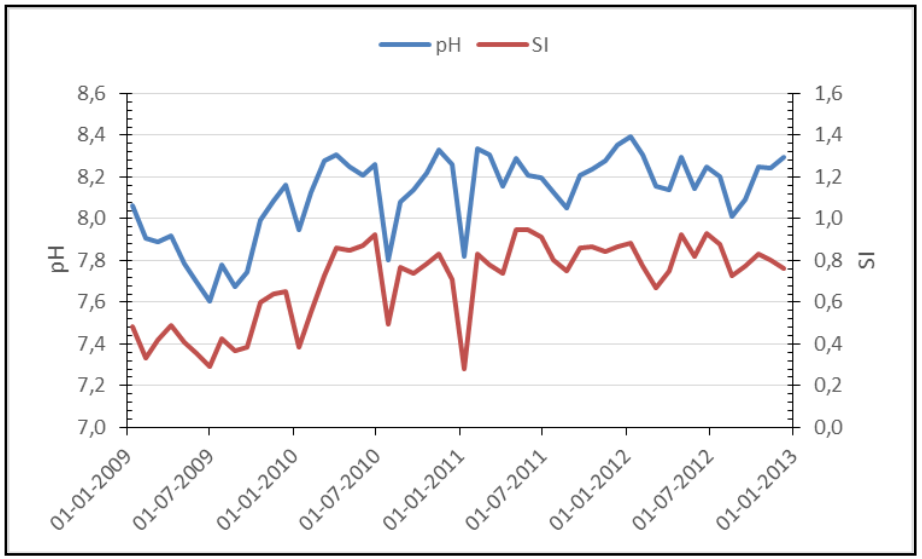


Calculated carbon dioxide concentration

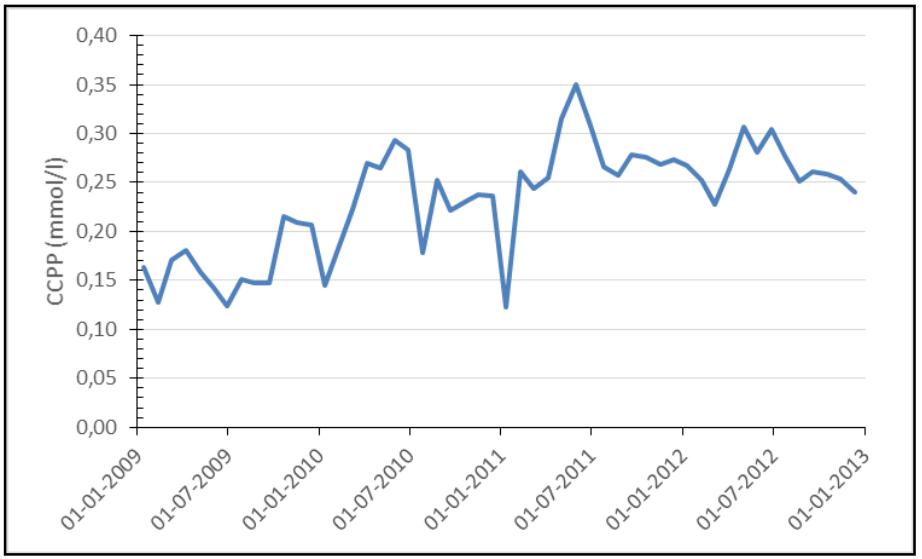
waternet

/innovation

Raw water evaluation with Stimela.dat



Calculated Saturation Index

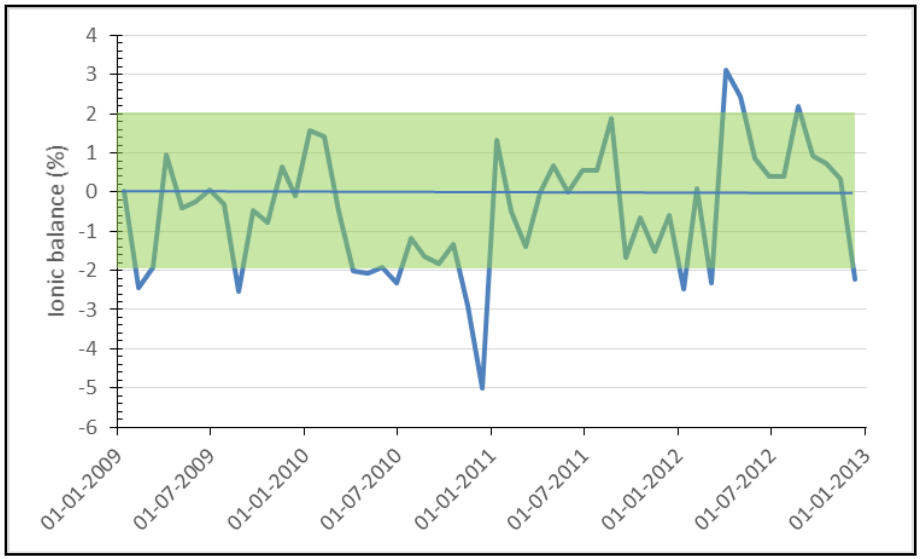


Calculated calcium carbonate precipitation potential

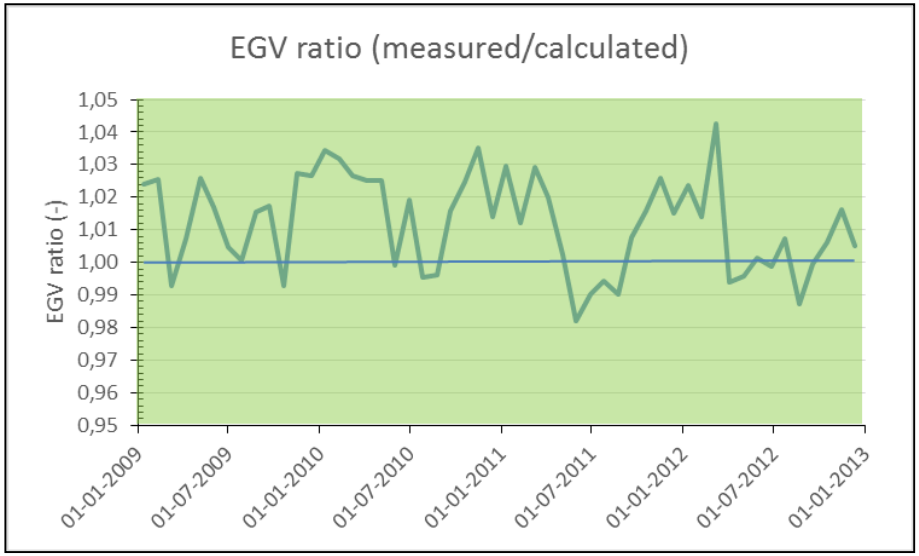
waterOnet

/innovation

Raw water validation with Stimela.dat



Calculated ionic balance

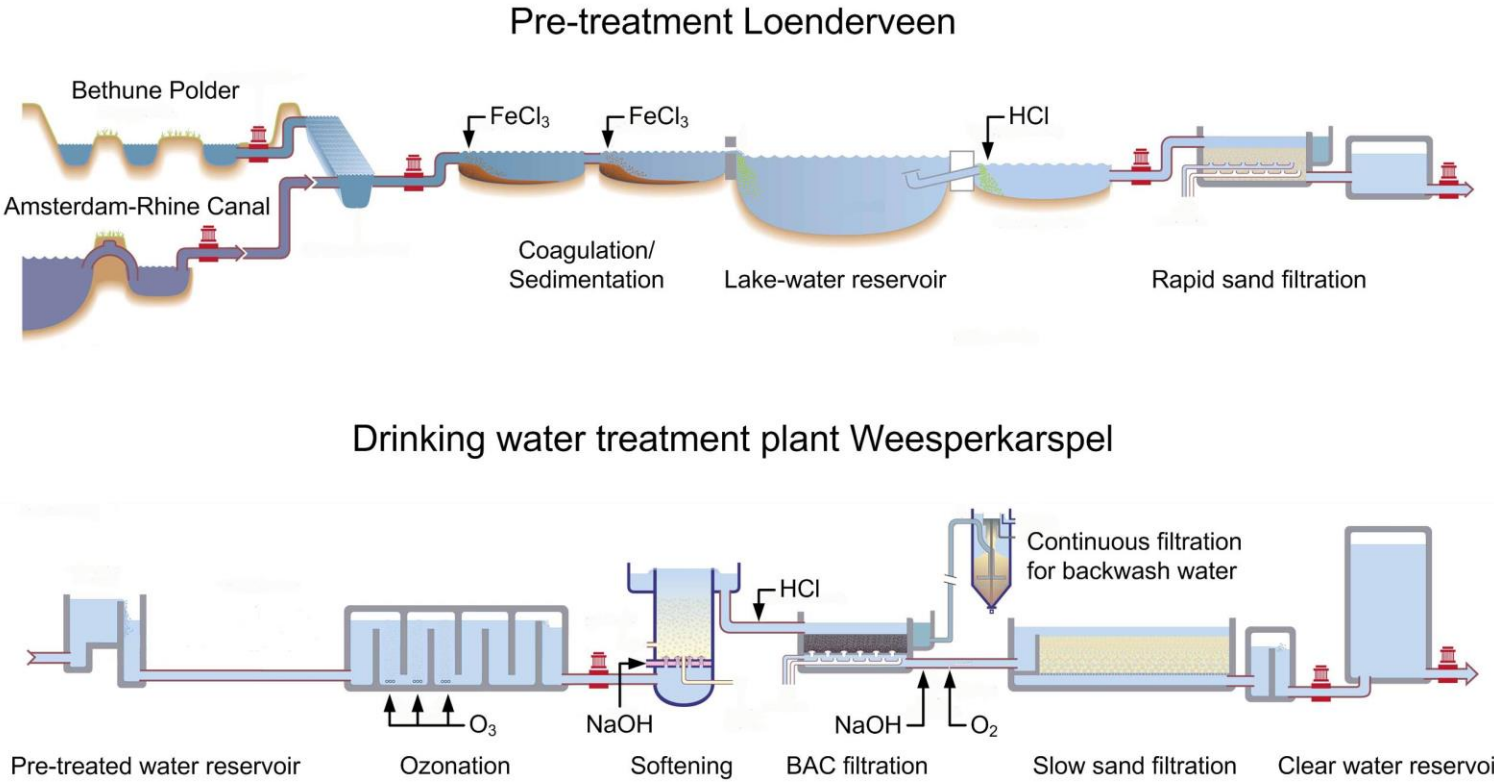


Calculated EGV ratio

waternet

/innovation

Treatment scheme



waterOnet

/innovation

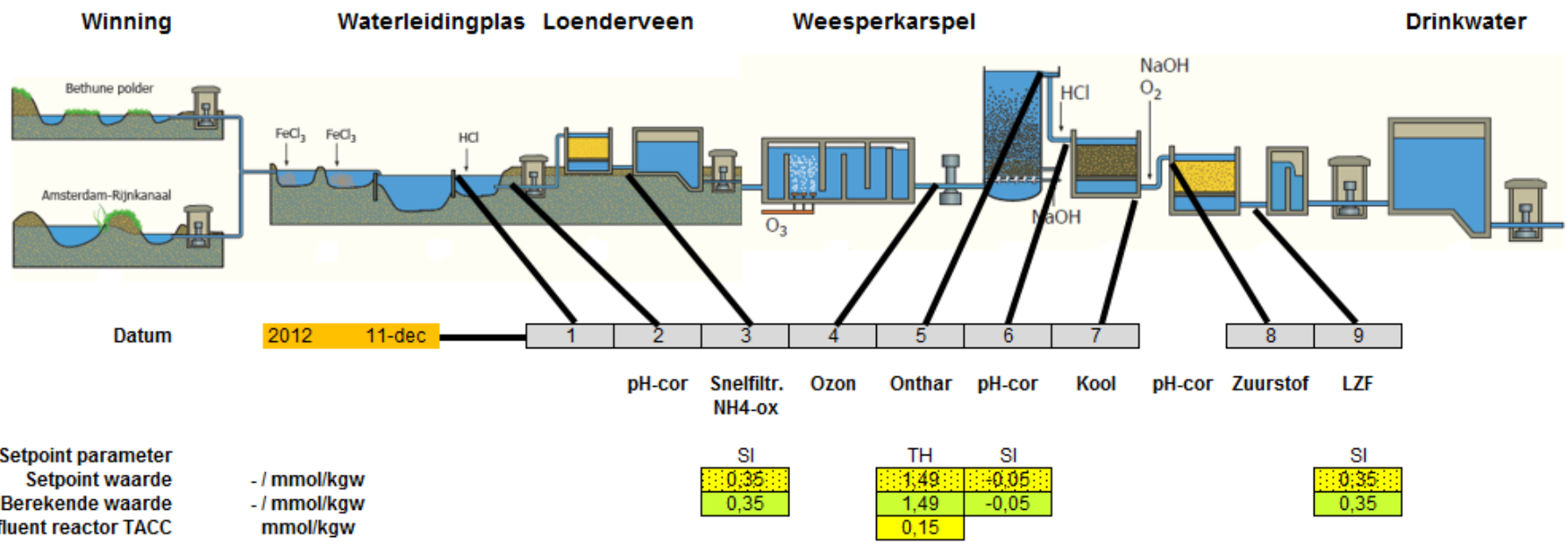
Modelled chemical processes

Process	Item	Reaction
pH control	HCl-dosing	$HCO_3^- + H^+ + Cl^- \rightarrow CO_2 + H_2O + Cl^-$
Filtration	NH_4-oxidation	$NH_4^+ + 2\ O_2 + 2\ HCO_3^- \rightarrow NO_3^- + 2\ CO_2 + 3\ H_2O$
Ozonation	O_3-reduction	$2\ O_3 \rightarrow 3\ O_2$
Softening	NaOH-dosing	$CO_2 + OH^- + Na^+ \rightarrow HCO_3^- + Na^+$
	NaOH-dosing	$HCO_3^- + OH^- + Na^+ \rightarrow CO_3^{2-} + Na^+$
	$CaCO_3$-crystallization	$Ca^{2+} + CO_3^{2-} \rightarrow CaCO_3(s)$
pH control	HCl-dosing	$CO_3^{2-} + H^+ + Cl^- \rightarrow HCO_3^- + Cl^-$
AC filtration	DOC-oxidation	$CH_2O + O_2 \rightarrow CO_2 + H_2O$
pH control	NaOH-dosing	$CO_2 + OH^- + Na^+ \rightarrow HCO_3^- + Na^+$
O_2 control	O_2-dosing	$O_2 \rightarrow O_2$
SS filtration	DOC-oxidation	$CH_2O + O_2 \rightarrow CO_2 + H_2O$

waterOnet

/innovation

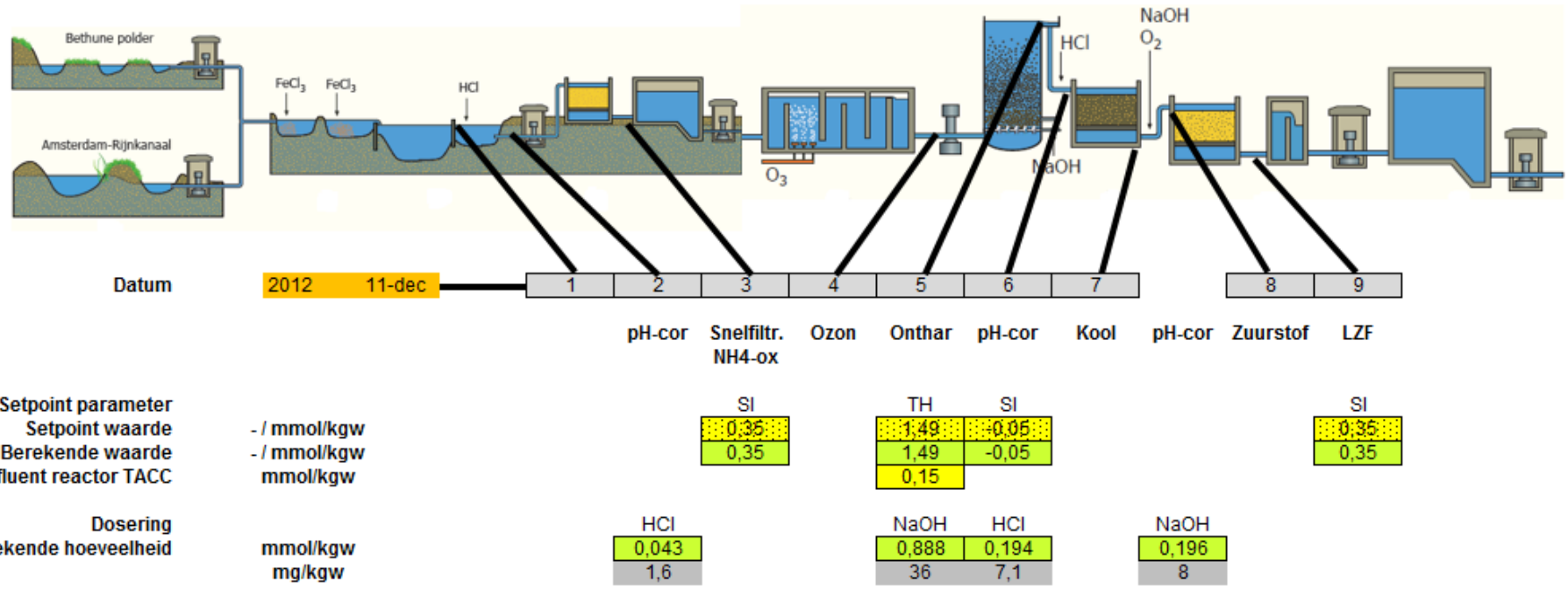
SI and Total Hardness (TH)



4 Setpoints in the treatment

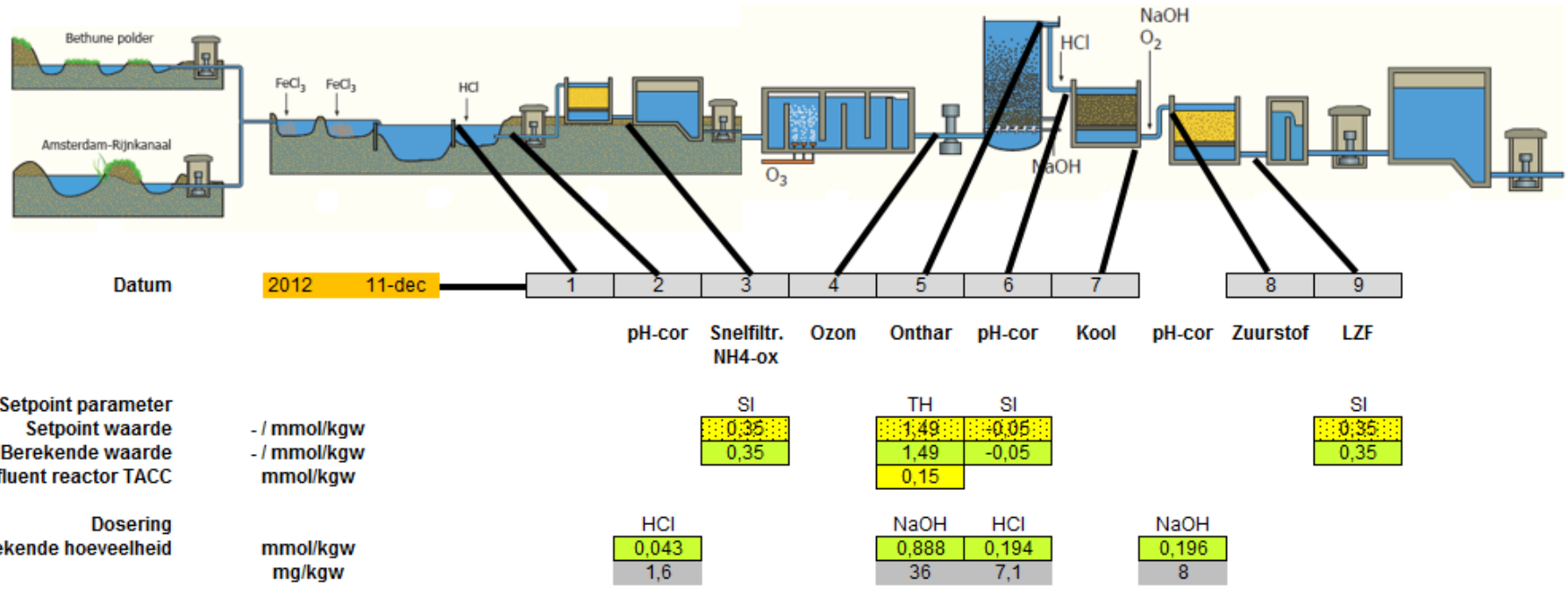
waterOnet

SI and Total Hardness (TH)



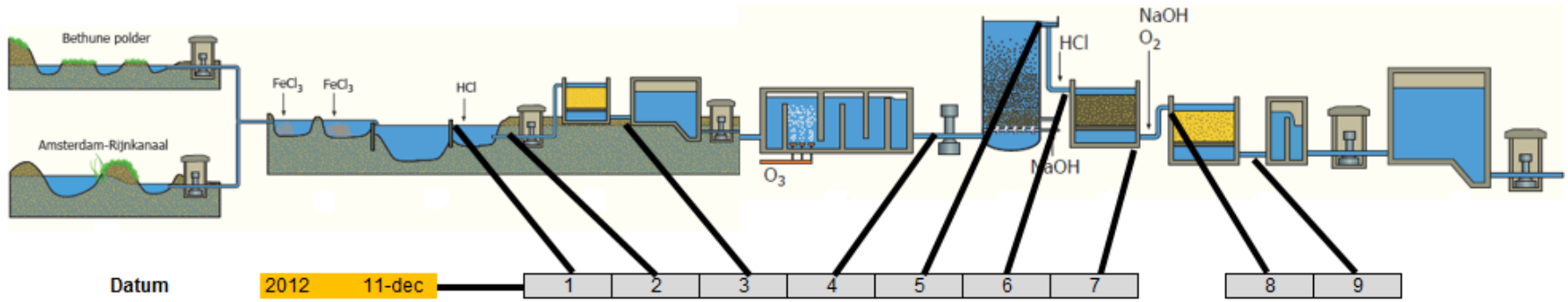
4 control points in the treatment

SI and Total Hardness (TH)



4 influencing processes in the treatment

SI and Total Hardness (TH)



Setpoint parameter			SI		TH	SI				SI
Setpoint waarde	- / mmol/kgw		0,35		1,49	-0,05				0,35
Berekende waarde	- / mmol/kgw		0,35		1,49	-0,05				0,35
Effluent reactor TACC	mmol/kgw				0,15					
Dosering		HCl			NaOH	HCl		NaOH		
Berekende hoeveelheid	mmol/kgw	0,043			0,888	0,194		0,196		
	mg/kgw	1,6			36	7,1		8		

Simulation with Stimela.dat

Run PHREEQC

/innovation

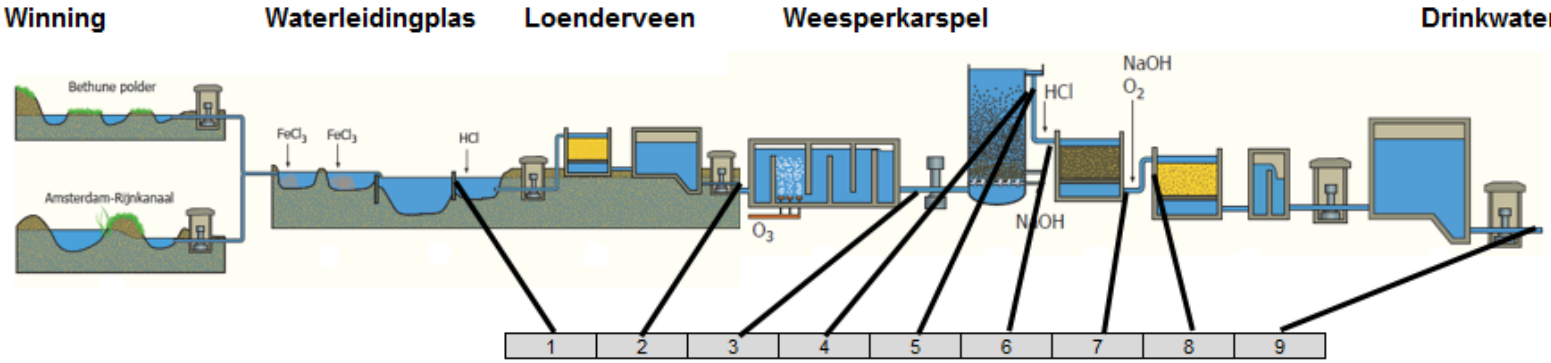
PHREEQC code in MS Excel

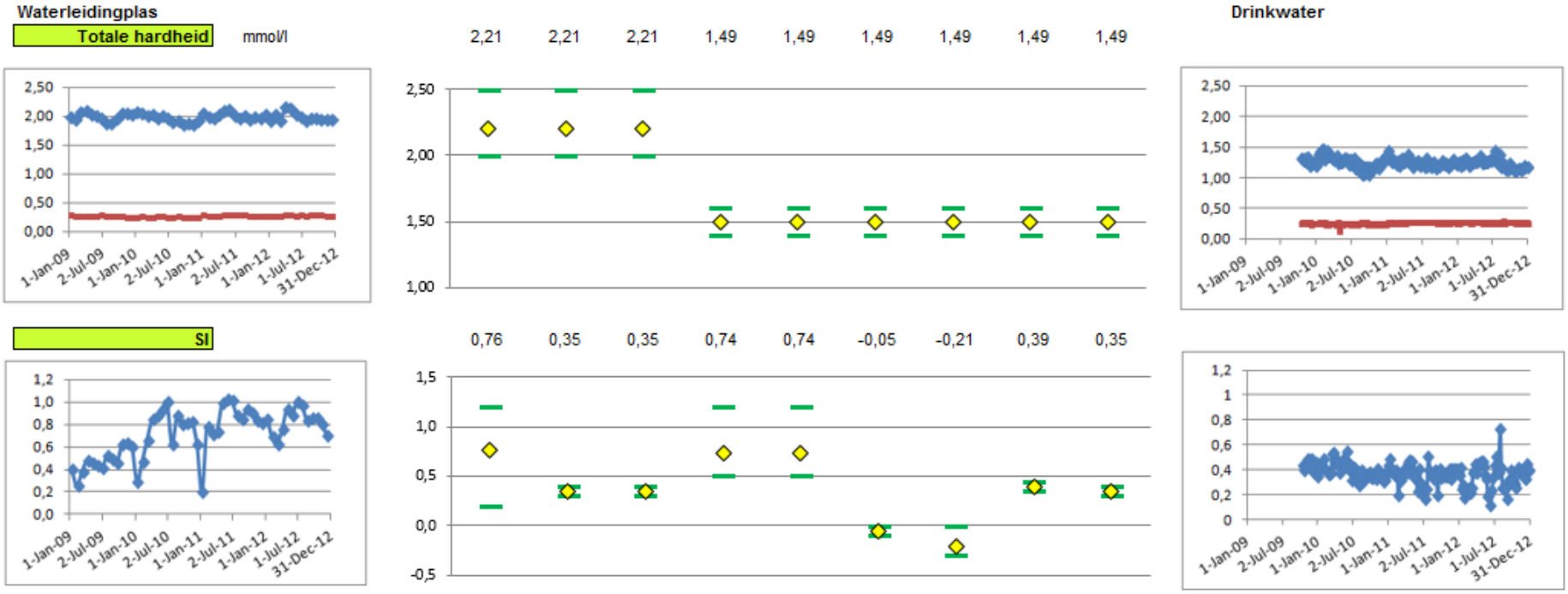
```
SOLUTION_SPREAD
        -units                  mg/L
        -redox                  O(-2)/O(0)              # if O2=0 then "pe" else "O(-2)/O(0)"
        -water                          1               # kg

number  temp            pH      Ca              Mg      Alkalinity      [N-3]   Na      K       Fe              Cl      S(6)    N(+5)   P       O(0)    Si      Org_c   density         Oxg     Ntg
                                as Ca           as Mg   as HCO3         as NH4  as Na   as K   as Fe           as Cl   as SO4  as NO3  as PO4  as O    as SiO2 as C
1       8,800           8,298   77,640          8,555   234,470         0,775   23,280  2,854   0,052           64,013  4,878   2,486   0,009   12,160  11,213  8,254   1,000324        1 Oxg(g) -( 1 Ntg(g)

END     # Simulation    1


TITLE   Berekening pe                    Batch-reaction for calculating pe (redox equilibrium) (dummy calculation)
        USE solution    1       ;       EQUILIBRIUM_PHASES 1;                                                   ; SAVE solution 2       ; END   # Simulati      2
TITLE   Berekening TACC / CCPP          Batch reaction for calculating CalciumCarbonate Precipitation Potential
        USE solution    2       ;       EQUILIBRIUM_PHASES 2;   Calcite                                                                 ; END   # Simulati      3


TITLE   Bepaling HCl dosering           Eerst reactie van NH4, daarna HCl dosering tot setpoint-SI, indien noodzakelijk (voorwaarde via comment marker #)
        USE solution    2       ;       REACTION;       [N-3]H4 -1 NH4 1;       0,042533        mmoles                  ; SAVE solution 22      ; END   # Simulati      4
        USE solution    22      ;       EQUILIBRIUM_PHASES 3; Calcite           0,3500  HCl             0,001                                   ; END   # Simulati      5
#       USE solution    22      ;       EQUILIBRIUM_PHASES 3;                                                                                   ; END   # Simulati      5

TITLE   HCl  dosering                   Berekende dosering = Cl (sim5-sim4) in mol/kgw  (voor CO2 :  ook onderdeel  Verbruik in Bedieningspaneel aanpassen)
        USE solution    2       ;       REACTION;       HCl     1;      0,0434  mmoles                  ; SAVE solution 3       ; END   # Simulati      6
        USE solution    3       ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      7

TITLE   Snelfiltratie - NH4 oxydatie    (zonder TOC omzetting)
        USE solution    3       ;       REACTION;       [N-3]H4 -1 NH4 1;       0,042533        mmoles                  ; SAVE solution 4       ; END   # Simulati      8
        USE solution    4       ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      9

TITLE   Ozon dosering                   (bijbehorende reacties zoals bromaatvorming niet gedaan)
        USE solution    4       ;       REACTION;       O3 1;           0,000000        mmoles                  ; SAVE solution 5       ; END   # Simulati      10
        USE solution    5       ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      11

TITLE   Ontharding - stap 1             Dosering en neerslag tot evenwicht
        PRINT; -selected_output false   # uitvoer naar Selected output UIT (tussenresultaten DoseTH niet nodig in Output)
        USE solution    5       ;       KINETICS ; DoseTH ; -formula    NaOH    1.0 ; -parms    1,3400  ; m0 10.0 ; -bad_step_max 100 ; -cvode true ; -steps 10 s in 10 steps
                                        EQUILIBRIUM_PHASES;     Calcite                                                 ; SAVE solution 6       ; END   # Simulati      12
        PRINT; -selected_output true    # uitvoer naar Selected output AAN (met alsnog uitvoer van laatste step)
        USE solution    6       ;       EQUILIBRIUM_PHASES;                                                                                     ; END   # Simulati      13

TITLE   Ontharding - stap 2             Toevoegen CaCO3 voor TTAC
        USE solution    6       ;       REACTION;       CaCO3 1;        0,1500  mmoles                  ; SAVE solution 7       ; END   # Simulati      14
        USE solution    7       ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      15

TITLE   HCl  dosering                   Zuurdosering tot setpoit SI                             (voor CO2 een andere Excel ontwikkelen)
        USE solution    7       ;       EQUILIBRIUM_PHASES 4 ; Calcite  -0,0500 HCl             10 ;                    ; SAVE solution 8       ; END   # Simulati      16
        USE solution    8       ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      17

TITLE   Koolfiltratie - TOC omzetting   TOC omzetting: Org_C + O2 --> CO2
        USE solution    8       ;       REACTION;       Org_c -1;       CO2 1;  O2 -1;  0,0781  mmoles                  ; SAVE solution 9       ; END   # Simulati      18
        USE solution    9       ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      19

TITLE   Bepaling NaOH dosering          Eerst reactie van TOC (vorming CO2), daarna NaOH dosering tot setpoint-SI
        USE solution    9       ;       REACTION;       CO2     0,0104  ; 1,00 mmol
                                        EQUILIBRIUM_PHASES 5 ; Calcite  0,3500  NaOH            0,001                                   ; END   # Simulati      20

TITLE   NaOH  dosering                  Berekende dosering = Na (sim20-sim19) in mol/kgw
        USE solution    9       ;       REACTION;       NaOH    0,1958  ; O2    0,0000  ; 1,00 mmol                  ; SAVE solution 10      ; END   # Simulati      21
        USE solution    10      ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      22

TITLE   Langzame zandfiltratie - TOC c  TOC omzetting: Org_C + O2 --> CO2
        USE solution    10      ;       REACTION;       Org_c -1;       CO2 1;  O2 -1;  0,0104  mmoles                  ; SAVE solution 11      ; END   # Simulati      23
        USE solution    11      ;       EQUILIBRIUM_PHASES;     Calcite                                                                 ; END   # Simulati      24
```

waterOnet

/innovation

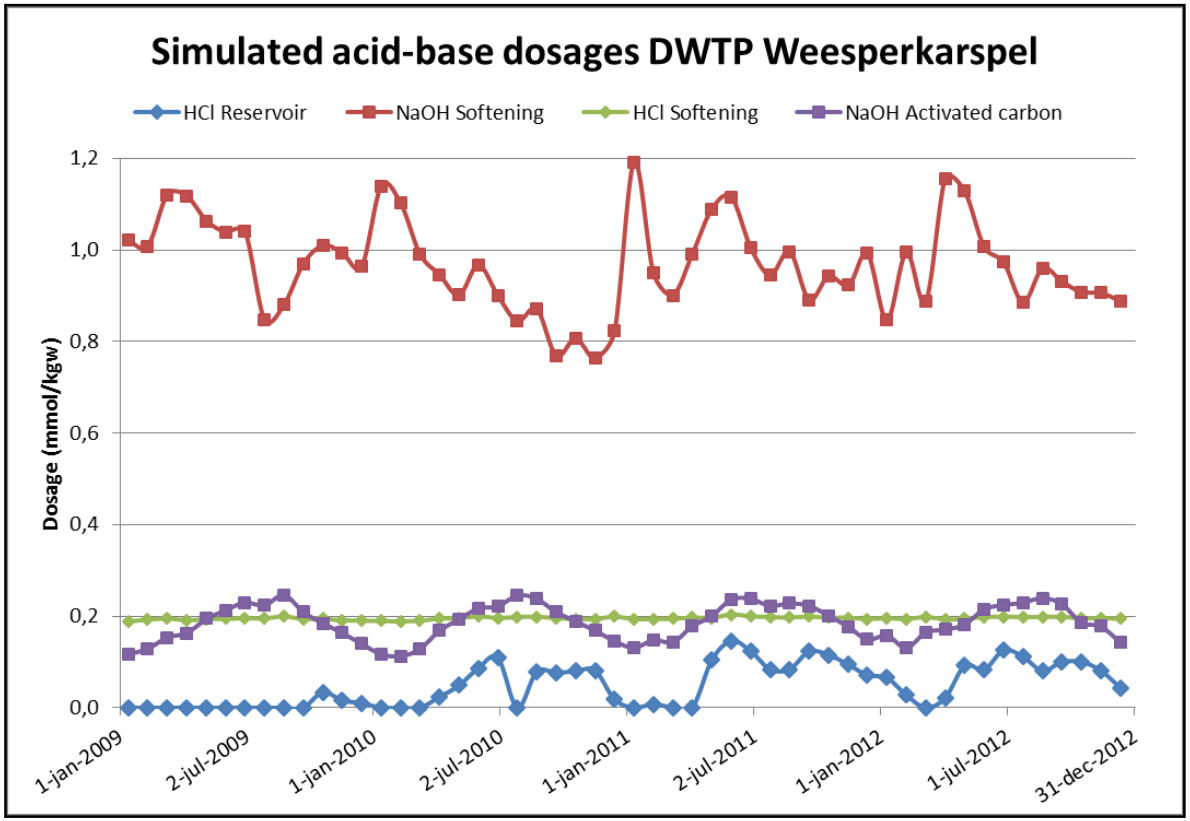
Results in process dashboard





/innovation

Multiple simulations

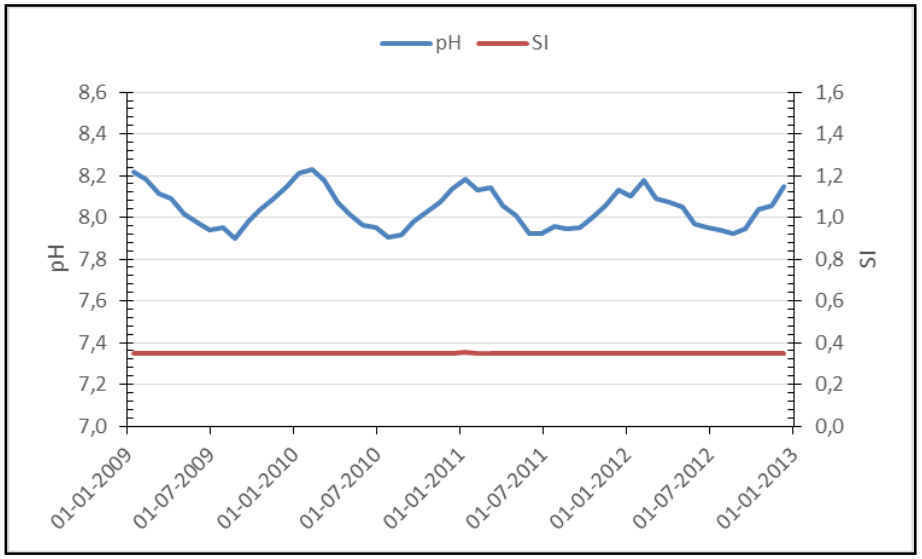


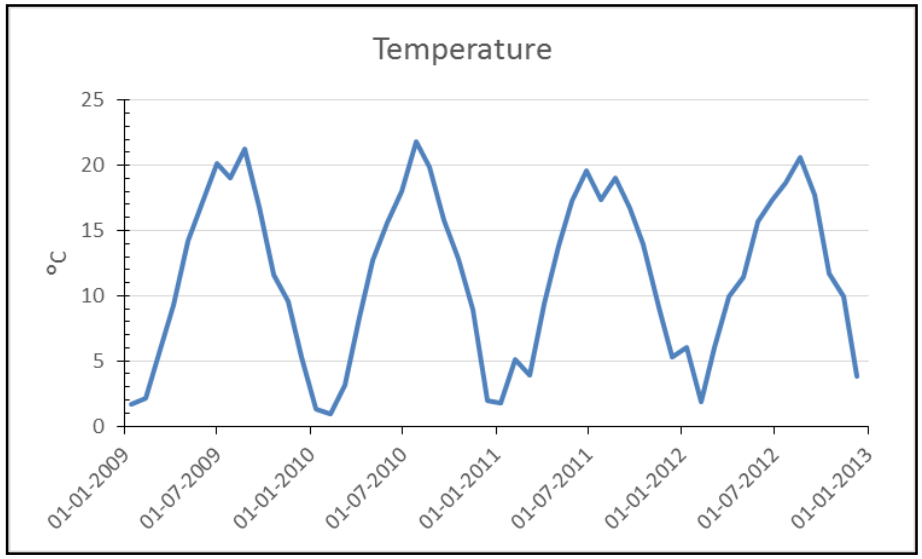
Long term process evaluation

waterOnet

/innovation

Multiple simulations





Effect on drinking water quality:

- Stable SI
- Slightly varying pH due to temperature

/innovation

Conclusions

- Accurate chemistry available for process technologists with Stimela.dat in PHREEQC
- Chemical dosages can be optimised
- Improving chemical stability of drinking water
- User interface simply build and adapted in MS Excel

/innovation

Plant wide chemical water stability modelling with PHREEQC for drinking water treatment

Alex van der Helm	Waternet / Delft University of Technology
Onno Kramer	Waternet
Jos Hooft	Waternet
Peter de Moel	Omnisys/ Delft University of Technology

2nd IWA New Developments in IT & Water Conference, Amsterdam, the Netherlands, February 10th 2015