

Customer case

How smart models helped to optimize Bayer's industrial wastewater treatment



Case highlights:

- Bayer wanted to minimise chemical dosing and sludge disposal by modifying their wastewater treatment process in Antwerp
- A smart combination of AM-Team's dynamic and CFD models were used for virtual technology assessment
- Models calibrated based on lab data were used to predict full-scale performance
- Virtual piloting replaced expensive onsite piloting at a fraction of the time and cost
- Process changes were successfully implemented at full scale
- Significant cost and sustainability benefits were obtained:
 - -40% NaOH dosing requirements
 - -35% sludge production (including savings of several hundreds of tons of chemicals per year)

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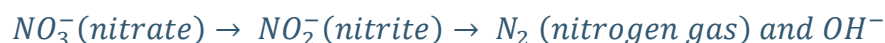
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Introduction and Problem statement

The life sciences enterprise Bayer provides products and services in the fields of healthcare and agriculture. As of December 31, 2024, the Bayer Group comprised 291 consolidated companies in 80 countries.

At their Bayer site in Antwerp (Belgium), 2 million m³ of wastewater gets treated every year. The treatment plant (Figure 1) consists mainly of a biodegradation basin with 3 consecutive compartments (with anoxic/aerobic/aerobic conditions), clarifiers and a dissolved air flotation unit. Bayer was assessing a process modification that showed the potential to significantly reduce chemical dosing requirements and sludge disposal of the wastewater treatment process. If successful, it would lead to major operational cost savings and sustainability gains.

Industrial wastewater treatment typically is characterised by a complex mixture of incoming wastewater streams to be treated. One of those streams at the Antwerp site is highly acidic and always had been neutralised completely through sodium hydroxide (caustic) dosing prior to entering the biological process. Bayer was investigating if this pH correction was essential as the biological treatment process could potentially take care of the neutralisation itself. As shown in Equation 1, the biological nitrogen removal process inherently produces hydroxide (OH⁻) which automatically drives up the pH.



Equation 1: Biological nitrogen removal relies on denitrification, in which bacteria convert nitrate in the wastewater (NO₃⁻) to harmless nitrogen gas (N₂) that leaves via the air. The hydroxide produced in that process will automatically elevate the pH.

In addition, relying on self-neutralisation would drive down the overall pH of the whole biological treatment, potentially avoiding significant sludge formation and related disposal costs from calcium carbonate (CaCO_3) precipitation. This is because at lower pH (<7.4) the equilibrium between $\text{CO}_2 \leftrightarrow \text{HCO}_3^- \leftrightarrow \text{CO}_3^{2-}$ shifts towards HCO_3^- , avoiding the precipitation of Ca^{2+} with CO_3^{2-} .

Bench-scale testing at the Bayer laboratory back in 2022 proved this self-neutralisation capacity, yet translation to dynamic full-scale conditions (i.e. translation from batch to continuous wastewater treatment) still needed to be made. AM-Team helped Bayer with translating the bench-scale insights to full scale operation by conducting virtual full-scale feasibility testing and model-based design of the actual process modification.

Key system characteristics

- Industrial wastewater treatment plant (classic activated sludge)
- Treatment lanes consisting of anoxic and aerobic compartments, followed by final clarifiers
- Aeration with pure oxygen
- Treatment of nitrate-rich acidic (pH 2.0) stream and 7 other industrial wastewaterstreams

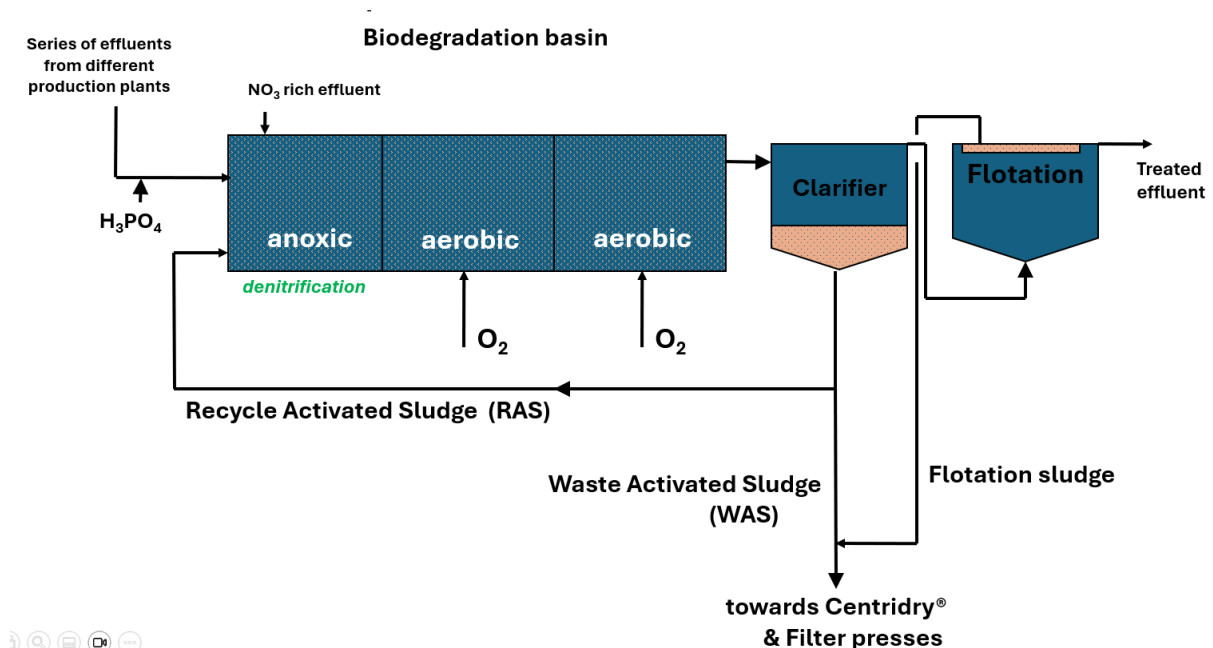


Figure 1: The wastewater treatment plant of Bayer in Antwerp (Belgium)

Solution and Objectives

Bayer relied on AM-Team's dedicated portfolio of treatment plant models to support the planning and design stage:

- In the planning stage, where the focus is on process concept evaluation and selection, virtual piloting offers nearly unprecedented testing freedom and significant cost and time savings compared to conventional onsite piloting.
- In the design stage, where the focus is on process concept implementation, model-based design assures maximum process performance and efficiency prior to construction.

The objectives of this project were to:

1. assess feasibility of the process modification at full-scale: translate Bayer's bench-scale tests to full-scale conditions using a dynamic model of the full-scale plant. Key questions included:
 1. Can neutralisation of the acidic stream be avoided or minimised, and would the resulting equilibrium pH and alkalinity still create viable conditions for the biological treatment process?
 2. Can CaCO_3 precipitation be avoided, driving down sludge disposal costs?
2. identify the optimal process design: make sure the upgrade can be implemented successfully using a detailed 3D simulation model that considers the critical process factors. Key questions included:

How to design the mixing system as such to minimise local toxicity in the biological process due to the low pH of the non-neutralised stream? (since Bayer's intensive bench-scale testing revealed the negative impact of suboptimal mixing of the acidic stream in the biodegradation basin on the life/death fractions of the micro-organisms)

"Knowing which model to apply when is what we like to call a 'model-fit-for-purpose' approach. A smart combination of models can dramatically increase the impact and business case of modelling. In this case, a combination of dynamic modelling with CFD proved to be highly effective."

- Roberta Muoio, ir., Senior Simulation Engineer,
AM-Team



Approach

AM-Team relied on its toolbox of different models tailored to treatment processes. In this case, a dynamic plant model and a 3D CFD model of the treatment process were used:

- The dynamic plant model included chemical and biological kinetics and hence could predict biological conversion, pH equilibrium and CaCO_3 precipitation under the dynamic conditions of the full-scale plant. This mode was used for the virtual piloting and feasibility testing.
- The bioreactor CFD model simulated the system in full 3D and accounted for the critical design elements and mixing of different flows. The real system geometry and even the rotation of the mixers could be easily taken into account. This model was used for the detailed design.

Both models hence were used to answer different questions related to planning and design. A multitude of 'what-if' scenarios were tested and compared using both models.

"The virtual scale-up of our batch results from the lab to our continuously-operated wastewater treatment plant was extremely important for our project. Once the models exist you have all flexibility to gain new insights. It is fascinating to see how your plant will operate at new conditions before these new conditions are actually in place! Compared to old-school 'real-live piloting' you can test much more with the 'virtual piloting' - and in a much more convenient way - which makes it an amazing optimization tool!"

- Bart Peeters, Dr. ir., Senior Expert Wastewater Treatment, Bayer



Results and findings

Bench-scale model: calibration based on available testing data

Bayer already performed bench-scale denitrification testing of the process modification (Figure 2a), thereby dosing hydrochloric acid to compensate for the pH increase during the denitrification, this way keeping the pH neutral in the bioreactor. The biological denitrification performance, pH and CaCO_3 precipitation were monitored across the different runs. In order to calibrate the dynamic model, the bench-scale tests were replicated with the model (Figure 2b). As such, the model could be calibrated for the specific biological sludge of Bayer's wastewater treatment plant using the already available data (Figure 2c). Biological kinetics, aeration, different carbon fractions, buffering capacity and precipitation reactions were all included in the model.

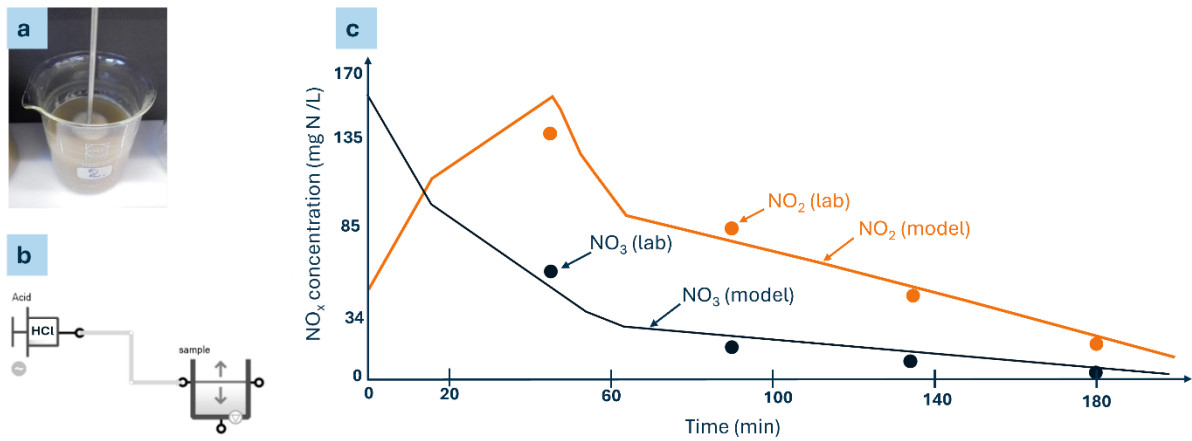


Figure 2: The real bench-scale denitrification tests performed by Bayer (a) were replicated with a virtual bench-scale model (b) to prepare the model for virtual full-scale assessment - dynamic profiles of nitrogen species (c) and pH were compared

Building and validating the full-scale model

Upon successful bench-scale calibration, the model of the full-scale wastewater treatment plant was configured (Figure 3a). The calibrated biological parameters obtained from the bench-scale modelling were used while the plant layout, volumes, flow rates and influent dynamics of the real full-scale were applied. As such, based on the bench-scale data, a calibrated full-scale plant model was obtained. As shown in Figure 3a (right), the secondary settler was also taken into account, allowing a realistic prediction of the activated sludge dynamics of the full-scale plant.

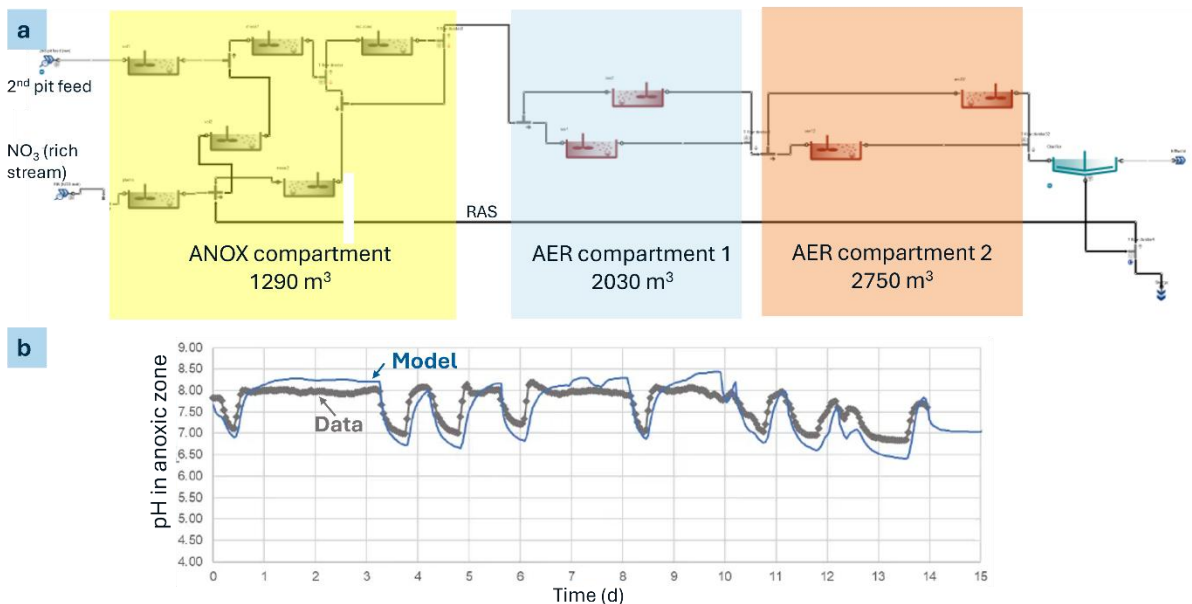


Figure 3: The model of Bayer's full-scale plant (a) included the real influent streams, operational settings, reactor volumes and settler. Model validation based on full-scale data showed satisfactory prediction of pH dynamics.

To validate the full-scale model, the normal operation (with usual pre-neutralisation of the acidic stream from pH 1.6 to 6.2) was first replicated with the model. Figure 3b shows the pH dynamics in the anoxic compartment for a period of 15 days. pH during normal operation usually fluctuated around 7.5. The model was adequately predicting the pH dynamics both in the anoxic zone and the final effluent (results of the latter not shown).

Virtual ‘what-if’ testing at full-scale

The model could now be used to conduct ‘what-if’ scenario tests that were impossible to conduct with the real full-scale plant. These scenarios would reveal the feasibility of the process change at full-scale. Three different scenarios were run in which the acidic stream was introduced directly in the anoxic zone while being partially neutralized to pH 2 and pH 1.85 compared to normal operation (i.e., complete neutralisation to pH 6.2). One of the scenarios also included an alternative aeration system including regular aeration next to the existing pure oxygen injection, and the resulting impact on the operational pH.

Figure 4 shows the summary and comparison of all scenarios in terms of resulting pH and alkalinity inside the bioreactor. Even with a partially neutralized wastewater at a pH 1.85 (scenario 3) the resulting pH of both anoxic zone and effluent was expected to stay well above 6.5, which was deemed acceptable for the biology. In addition, alkalinity stayed above reasonable levels to still create favourable conditions.

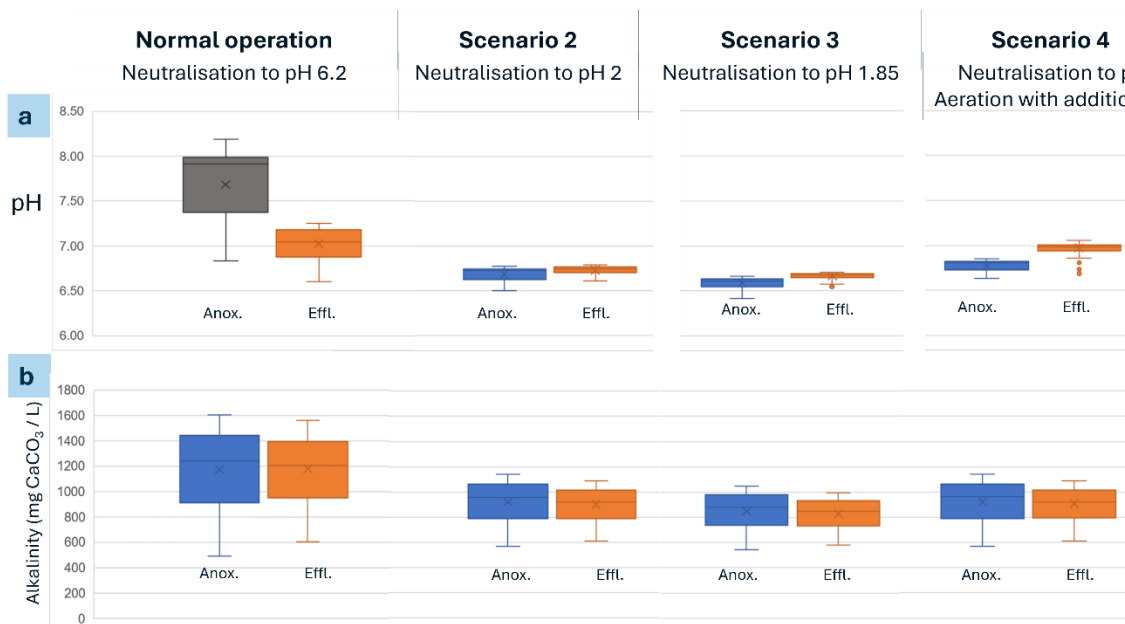


Figure 4: Compared to normal operation, direct introduction of the acidic stream with a significantly reduced neutralisation degree drives down the pH in the bioreactor, especially in the anoxic zone (a), yet pH stabilises at acceptable levels (>6.5) in all scenarios due to the self-neutralisation capacity of the anoxic zone. Also alkalinity drops but stays at acceptable levels.

The model simulations revealed a significant impact on sludge disposal costs: due to the operation at lower pH and resulting higher solubility of CaCO_3 , the CaCO_3 mass in the waste sludge was expected to drop from 3 kg/m^3 sludge to negligible levels.

As a result of the full-scale feasibility testing, Bayer decided to immediately pursue full-scale implementation.

“The use of models to reduce or replace onsite piloting is what we refer to as ‘virtual piloting’. It leads to significant cost and time savings, while virtual testing freedom is nearly unlimited. Virtual piloting is possible as we combine years of modelling experience with high-quality models.”

- Roberta Muoio, ir., Senior Simulation Engineer,
AM-Team



Full-scale implementation and operation

Even though the virtual feasibility testing from a process standpoint was positive, the actual full-scale mixing system still needed to be designed. In this design stage, AM-Team applied a 3D CFD model that allowed for detailed assessment of mixing device placement.

The key of successful implementation was in rapidly mixing the acidic stream (pre-mixed with another neutral wastewater to a pH of about 4.5) with the bulk volume of the anoxic tank, as such to minimise local ‘low pH toxicity’ (minimize contact-time of the micro-organisms to toxic pH). Bayer’s batch testing already revealed potential toxicity under suboptimal mixing conditions. Given their experience with Ventoxal units (Air Liquide), these devices were considered by Bayer as an innovative way to introduce the acid wastewater into the biological compartment, and, hence, the Ventoxal units were included in the CFD runs.

5 scenarios with varying placements of the Ventoxal units were simulated and compared based on the predicted volume of the ‘low pH plume’, caused by the introduction of the acidic stream (Figure 5a). The objective was to minimise this volume.

While it became clear that the Ventoxal mixing device could significantly accelerate mixing compared to the initial design with a pipe inflow (‘current design’), further optimisation was possible by mounting the unit vertically at one of the reactor walls, thereby injecting under an angle in the opposite direction of the outlet (Figure 5b). This design, further referred to as ‘design 5’, led to a minimal toxicity risk and superior mixing (Figure 5c).

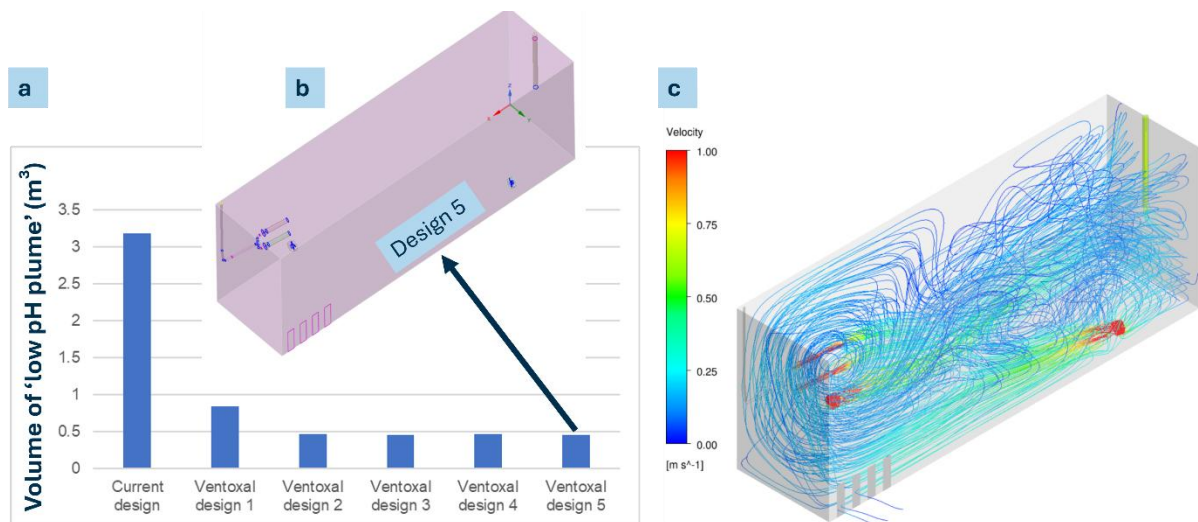


Figure 5: Introducing the acidic stream in the anoxic tank using a rapid mixing unit (Ventoxal) proved critical (a). Compared to regular introduction with a pipe ('current design'), rapid mixing drastically decreased the volume of the 'low pH plume'. Mounting the mixing unit vertically at the side wall, positioned under a slight angle (design 5; b) led to the the fastest mixing (c).

As a result, Bayer pursued onsite implementation of 'design 5' (Figure 6) in the anoxic compartment of its biodegradation basin.



Figure 6: The Ventoxal mixing units were placed in accordance with the most optimal CFD scenario. This design, with a specific vertical placement of the mixing units, was expected to create minimal low-pH toxicity.

“Let’s be honest, to finally take the plunge to implement the idea of self-neutralizing nitric acid wastewater was not straightforward at all. It was a bit ‘tricky’ as we say, since dealing with living organisms at risk for the lower pH conditions. Partly thanks to the low-pH plume modelling of AM-Team we were confident that the real-live implementation would be a success”

- Bart Peeters, Dr. ir., Senior Expert Wastewater Treatment, Bayer



Bayer started operating the newly configured system in October, 2024, thereby gradually decreasing the neutralisation of the acidic stream. By April 2025, the incoming pH already dropped to 2.2, resulting in a pH in the anoxic zone (Figure 7a) of around 6.9. This was perfectly in line with the predictions from the virtual feasibility assessment (see earlier).

The significant drop in inorganic sludge fraction (caused by CaCO_3 precipitation) also became visible (Figure 7b), with a drop from 45% to 12%. As a result of the avoidance of the higher-density CaCO_3 precipitation, sludge settleability deteriorated, but still stayed within acceptable levels.

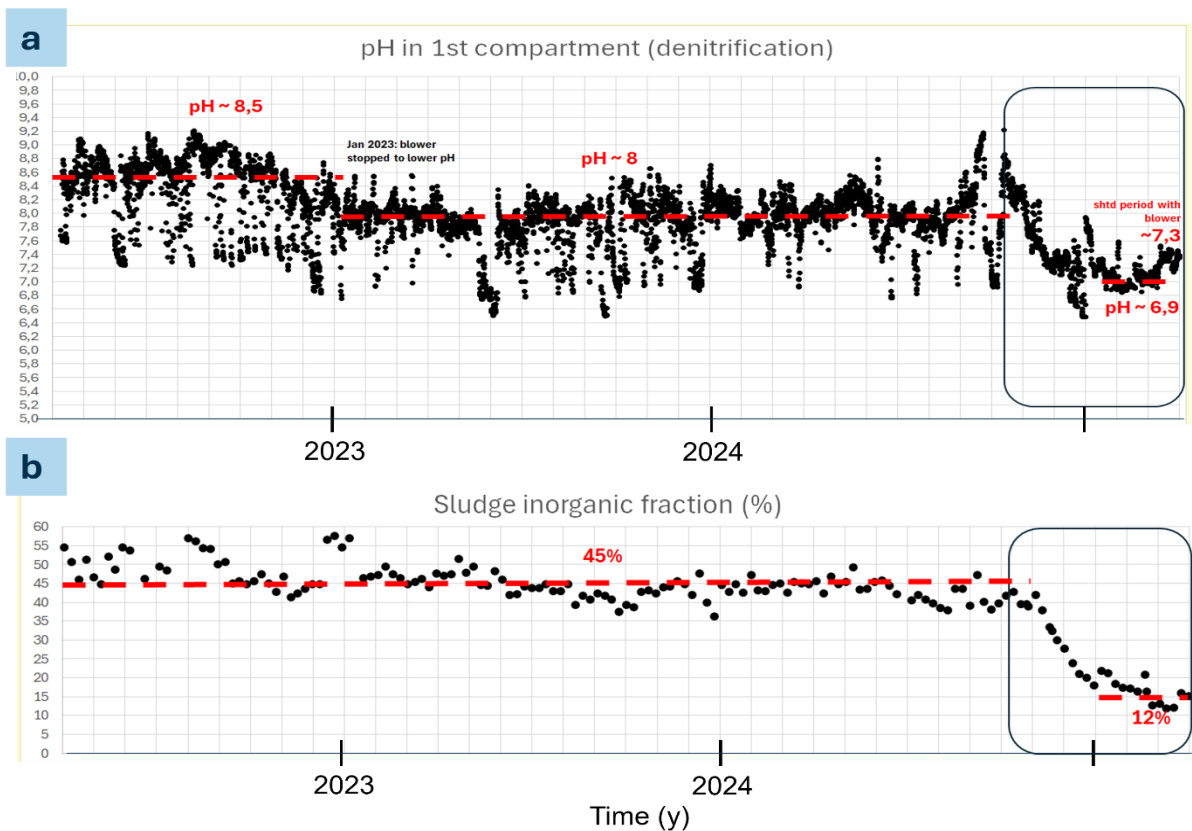


Figure 7: The updated process is in operation since October, 2024, with gradual decrease in acidic feed stream neutralisation. The change is very successful with operational pH at the levels predicted by the model, significant drops in sludge disposal costs and a significant saving of external caustic.

Conclusion and impact

Bayer could in Antwerp dramatically accelerate a full-scale process assessment and implementation using a smart combination of models:

- Virtual piloting instead of physical onsite piloting
 - Calibrated on real bench-scale data, a dynamic full-scale plant model could completely replace expensive and extensive onsite piloting. In addition to the associated cost and time savings, a multitude of scenarios could be assessed, offering nearly unlimited testing freedom compared to physical piloting. The latter offered significant additional confidence.
- Model-based process design
 - A detailed CFD model was used to optimally design the mixing system essential for the process modification. The potential negative impact of local low-pH toxicity on the biological treatment could be reduced to the utmost minimum. The best design scenario was meticulously implemented in practice.

Bayer's process experience and expert knowledge combined with AM-Team's modelling capabilities led to an innovative, successful process update with significant cost and sustainability benefits associated to sludge disposal and chemical use: (i) the acidic wastewater stream is only partially neutralized now, reducing the NaOH requirements for neutralization with 40% and (ii) the sludge generation at the wastewater treatment was reduced with 35% having a huge effect on the sludge handling costs (including a reduction in dewatering additives per year amounting to several hundreds of tons of chemicals).

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About AM-Team :

AM-Team provides globally unique modelling and data services and digital twin solutions to smartly design, optimise and digitalise municipal and industrial water and wastewater treatment plants. The company has worked on over 150 sites on 4 continents. AM-Team directly works with utilities and also partners with engineering firms, software companies and technology vendors.

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