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Modelling future levels of nitrosamines and nitramines in a groundwater compartment close to a CO₂ capture facility



REPORT

Main Office

Økernveien 94
NO-0579 Oslo, Norway
Phone (47) 22 18 51 00

NIVA Region South

Jon Lilletuns vei 3
NO-4879 Grimstad, Norway
Phone (47) 22 18 51 00

NIVA Region East

Sandvikaveien 59
NO-2312 Ottestad, Norway
Phone (47) 22 18 51 00

NIVA Region West

Thormøhlensgate 53 D
NO-5006 Bergen Norway
Phone (47) 22 18 51 00

NIVA Denmark

Njalsgade 76, 4th floor
DK 2300 Copenhagen S, Denmark
Phone (45) 39 17 97 33

Internet: www.niva.no

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Author(s) Cathrine Brecke Gundersen, Magnus Norling, Ashenafi Seifu Gragne	Topic group Environmental contaminants - freshwater	Distribution confidential
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<p>Summary</p> <p>Future levels of the carcinogenic and potentially carcinogenic nitrosamines (NSAs) and nitramines (NAs), respectively, were modelled in two water protection aquifers, Ramlösa Hälsobrunn and Åstorp, considering amine-based CO₂ capture at the nearby Filborna EfW plant. A high-resolution and dynamic catchment model (INCA-Contaminants) was used. NSA and NA deposition rates (provided by Norsk Energi) were combined with site specific information (hydrology and climate), and literature values of NSA and NA physiochemical properties and degradation rates. Water residence time and NSA and NA biodegradation half-lives were found to be the most uncertain and influential parameters. At both sites, NSA and NA levels are likely to remain below the recommended safety limit (4 ng L⁻¹), but care should be taken due to the uncertainty of the half-life. At Åstorp, additional uncertainty is associated with the result due to the uncertain water residence time of the aquifer.</p>
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Project Manager/Main Author

Cathrine Brecke Gundersen

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Hans Fredrik Veiteberg Braaten

Preface

The catchment modelling to estimate future concentrations of nitrosamines (NSAs) and nitramines (NAs) in two groundwater basins was conducted by the Norwegian institute for Water Research (NIVA) on commission from Öresundskraft Kraft & Värme AB. Ann-Sofie Lindqvist was the contact person for the project. Dag Borgnes from Norsk Energi provided the data from the atmospheric dispersion and deposition modeling.

At NIVA, the catchment modelling was conducted by Magnus D. Norling. Cathrine Brecke Gundersen was the project manager and contributed with expertise in the catchment processing of NSAs and NAs. Ashenafi Seifu Gragne contributed with data and expert evaluation regarding the groundwater basins. Data contribution was also made by Areti Balkoni. Thank you to Rolf D. Vogt for input regarding water chemistry.

François Clayer was responsible for the quality assurance of the results.

Oslo, 12.02.2024

Cathrine Brecke Gundersen

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Summary

Technology for CO₂ capture is an important mitigation option for CO₂-intensive processes like waste incineration. While intended to do good for the global climate, it is vital that implementation proceeds with minimal negative impacts on the local environment. The currently most feasible technique for capturing CO₂, using amines, is associated with risk of forming carcinogenic and potentially carcinogenic nitrosamines (NSAs) and nitramines (NAs), respectively. The formation occurs in the atmosphere, from amines unintentionally escaping the capture plant with the scrubbed flue gas. Drinking water reservoirs are of particular concern for receiving NSAs and NAs. The Norwegian Institute for Public Health (NIPH) has issued a recommended drinking water safety limit at 4 ng L⁻¹ for the sum of NSAs and NAs. A corresponding limit has to date not been established in Sweden.

Implementation of CO₂ capture is underway at the Filborna EfW plant (Öresundskraft Kraft & Värme AB) in Helsingborg, Sweden. As part of their environmental assessment, atmospheric dispersion and deposition modelling has already been carried out, finding two water protection areas, the Ramlösa Hälsobrunn and Åstorp to likely receive the highest deposition rates of NSAs and NAs.

The aim of this study was to assess the water concentration of NSAs and NAs in the two aquifers, considering CO₂ capture at the nearby Filborna EfW plant. The results were evaluated against the NIPH drinking water limit. A time period of more than 100 years was modelled to assess the potential for accumulation with time. This was achieved using the INCA-Contaminants catchment model (INCA-Tox). Deposition rates for NSA and NA (provided by Norsk Energi) were combined with site specific information (hydrology and climate), and literature values for NSA and NA physiochemical properties and degradation rates. At both sites, the most uncertain and influential parameter was the NSA and NA biodegradation half-life. The likely ranges were set to between 2 and 10 years. Studies assessing the biodegradability of relevant NSAs and NAs are scarce, and thus the set parameter values are associated with relatively high uncertainty. At Åstorp, also the water residence time was uncertain (5-20 years). To encompass the uncertainty of these two parameters, several different scenarios were simulated within their extreme values.

Results showed that future levels of NSAs and NAs were likely to remain below the safety limit at both two sites. At Ramlösa Hälsobrunn this was achieved with a half-life of 10 years and a residence time at 65 years. Pushing the extreme of the half-life, beyond what here is considered likely, a parameter value of 22 years would result in the safety limit being exceeded. At the Åstorp groundwater basin the situation was less clear. This was caused by a shorter anticipated residence time which has not been precisely determined. A lower residence time typically results in higher contaminant concentrations, which in turn is more sensitive to uncertainty in the biodegradation half-life (with regards to the safety limit). The ranges of likely values for water residence time and biodegradation half-lives suggests that the concentration at Åstorp will stabilise between 1.0 to 3.2 ng L⁻¹.

In the entire chain of calculations, from atmospheric dispersion and deposition modelling to catchment modelling, worst case scenarios are applied at every uncertain parameter. However, still, uncertainty is associated with several of the set parameter values. Future research work should focus on reducing the uncertainty of key parameters such as water residence time and NSA and NA biodegradation.

Sammanfattning

Tittel: Modellerade framtida nivåer av nitrosaminer och nitraminer i två grundvattenreservoarer nära en CO₂-avskiljningsanläggning

År: 2023

Forfatter(e): Cathrine Brecke Gundersen, Magnus Norling, and Ashenafi Seifu Gragne

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Teknik för CO₂-avskiljning är en viktig åtgärd för att minska CO₂-utsläpp från avfallsförbränning. Även om det är avsett att gynna det globala klimatet, är det avgörande att implementeringen sker med minimal negativ påverkan på den lokala miljön. Den för närvarande mest genomförbara tekniken för att fånga CO₂, som använder aminer, är förknippad med risk för bildning av cancerframkallande och potentiellt cancerframkallande nitrosaminer (NSAs) och nitraminer (NAs). Bildningen sker i atmosfären, när aminer oavsiktligt släpps ut från avskiljningsanläggningen tillsammans med den rena rökgasen. Tillförelse av NSAs och NAs till dricksvattenreservoarer är särskilt oroande. I Norge har Norges institut för folkhälsa (NIPH) fastställt ett rekommenderat gränsvärde för dricksvatten på 4 ng L⁻¹ för summan av NSAs och NAs. Ett motsvarande gränsvärde har inte fastställts i Sverige.

Öresundskraft Kraft & Värme AB planerar för installation av CO₂-avskiljning på Filborna avfallsförbränningsanläggning i Helsingborg, Sverige. Som en del av deras miljöbedömning har modellering av atmosfärisk spridning och deposition av nitrosaminer och nitraminer genomförts (spridnings- och depositionsberäkningar aminer utförd av Norsk Energi). Resultaten visar att två vattenskyddsområden, Ramlösa Hälsobrunn och Åstorp, sannolikt kommer att få de högsta depositions hastigheterna av NSAs och NAs.

Syftet med denna studie var att utvärdera vattenkoncentrationen av NSAs och NAs i de två akvifererna, med hänsyn till CO₂-avskiljning vid den närliggande Filborna avfallsförbränningsanläggningen. Resultaten utvärderades mot NIPHs gränsvärde för dricksvatten. En tidsperiod på över 100 år modellerades för att bedöma potentialen för ackumulering över tid. Detta utfördes med hjälp av avrinningsområdesmodellen INCA-Contaminants (INCA-Tox). Depositionshastigheter för NSA och NA (tillhandahållna av Norsk Energi) kombinerades med platspecifik information (hydrologi och klimat) samt litteraturvärden för NSAs och NAs fysikaliska och kemiska egenskaper samt nedbrytningshastigheter. Vid båda platserna var den mest osäkra och inflytelserika parametern NSAs och NAs halveringstid för biologisk nedbrytning. De mest sannolika intervallerna sattes till mellan 2 och 10 år. Studier som fastställer biologisk nedbrytning av relevanta NSAs och NAs är få, och därför är de angivna parameter-värdena förknippade med relativt hög osäkerhet. Vid Åstorp var även uppehållstiden för vattnet osäker (5-20 år). För att inkludera osäkerheten hos dessa två parametrar simulerades flera olika scenarier inom deras extrema värden.

Resultaten visade att framtida nivåer av NSAs och NAs sannolikt kommer att understiga det norska gränsvärdet vid båda platserna. Vid Ramlösa Hälsobrunn uppnåddes detta med en halveringstid på 10 år och en uppehållstid på 65 år. Genom att öka halveringstiden, bortom vad som här anses troligt, skulle ett parametervärde på 22 år resultera i att gränsvärdet överskrids. Vid Åstorps grundvattenmagasin var resultatet mer osäkert. Detta berodde på en kortare förväntad uppehållstid för grundvattnet, vilken inte har bestämts med precision. En kortare uppehållstid resulterar vanligtvis i högre koncentrationer av föroreningar, vilket i sin tur gör att resultatet är mer känsligt för osäkerhet i halveringstiden för biologisk nedbrytning (med avseende på gränsvärdet). Intervallerna för sannolika

värden för uppehållstid och halveringstider för biologisk nedbrytning tyder på att koncentrationen i Åstorp kommer att stabiliseras mellan 1,0 och 3,2 ng L⁻¹.

I hela kedjan av beräkningar, från atmosfärisk dispersion och depositionsmodellering till avrinningsområdesmodellering, tillämpas värsta tänkbara scenarier för varje osäker parameter. Ändå finns det fortfarande osäkerhet förknippad med flera av de angivna parameter-värdena. Framtida forskningsarbete bör fokusera på att minska osäkerheten för nyckelparametrar som vattenresidens-tid och biologisk nedbrytning av NSA och NA.

1 Introduction

Implementation of CO₂ capture technology is key to limit global warming to below 1.5 °C by 2100 (IPCC, 2014). The technology can aid in the transition towards a low-emission, renewable energy dominated society and is currently the only option to drastically reduce emissions from CO₂-intensive processes like waste incineration and cement production (Bosoaga et al., 2009; Wienchol et al., 2020). While the intention is good for the global climate, we must ensure that implementation proceeds with minimal negative impact on human health and the local environment.

Associated with the currently most feasible technique for capturing CO₂ (using amines) is the risk of forming carcinogenic and potentially carcinogenic nitrosamines (NSAs) and (NAs), respectively (Chen et al., 2018; Reynolds et al., 2012). This occurs as small amounts of the amines used in the capture process will unintentionally escape from the capture plant with the cleaned flue gas. In the atmosphere, the amines will rapidly degrade to form NSAs and NAs, amongst other products. The reaction is initiated by sunlight and requires NO_x to proceed (Nielsen et al., 2012). Different compounds of NSAs and NAs will form depending on the type(s) of amines used in the capture process. Molecules of NSAs and NAs are considered hydrophilic and thus tend to be in the water phase. Thus, there is risk of NSAs and NAs contamination in drinking water reservoirs. The Norwegian Institute for Public Health (NIPH) has issued a recommended drinking water safety limit at 4 ng L⁻¹ for the sum of NSAs and NAs (and at 0.3 ng m⁻³ in air) (Låg et al., 2011). The limit is considered conservative since it is set based on the carcinogenicity of the most potent NSA (N-nitrosodimethylamine, NDMA). Other NSAs and NAs are expected to be less carcinogenic, but few studies exist to validate this. A corresponding safety limit has not to date been established by the Swedish authorities.

The company, Öresundskraft Kraft & Värme AB, plans to install CO₂ capture at their Filborna EfW plant, located in Helsingborg, Sweden (Figure 1). As part of their environmental assessment, potential effects from the amine technology are being assessed. To foresee whether the activities at a CO₂ capture plant can cause levels of NSA and NA in a nearby water compartment to exceed the safety limit, several complex processes must be considered. Atmospheric dispersion and deposition modelling has already been carried out. While the resulting air concentrations were not of concern, some of the highest deposition rates were identified over two water protection areas: the recharge zones of groundwater basins at Ramlösa Hälsobrunn and Åstorp (see Figure 1). Further investigations into resulting groundwater NSAs and NAs concentrations was warranted.

Once the NSAs and NAs are deposited on ground, a set of complex processes will interplay to govern final groundwater concentrations, which can be simulated using a catchment model. The physiochemical properties of the compounds govern their partitioning between air, soil, and water. The hydrophilic nature of the NSAs and NAs imply dominance in the aqueous phase. This is further supported by a low soil sorption potential (Gundersen et al., 2017; Gunnison et al., 2000). The NSAs are slightly more volatile than the NAs, so that a small fraction of the NSAs may escape from the water to the air. The NSAs and NAs remaining in the water phase will be percolated down to the groundwater.

Further governing the final groundwater NSA and NA concentrations are various degradation processes. For example, the NSAs will rapidly degrade under the exposure to sunlight, while this is not the case for the NAs (Sørensen et al., 2015). Biodegradation is another potential depletion pathway that can be of importance for the NSAs and NAs, and particularly under dark conditions where photodegradation of the NSAs cannot take place (e.g., in a groundwater basin). Only a few studies have so far investigated the biodegradability of NSAs and NAs relevant to CO₂ capture. In a recent study,

Brakstad et al. (2018) found that NSAs and NAs with an alcohol functional group (NDELA, MEA-NO₂ and AMP-NO₂)¹ were biodegradable in lake water (half-life from 28.2 to 35.1 days), and that a few NSAs and NAs were biodegradable under oxygen depleted conditions (NDELA, DMNA, and MEA-NO₂, half-life from 14 to 181 days). Some NSAs (NDMA and NPz)¹ and NAs (MNA, DENA, and Pz-NO₂)¹ did not biodegrade under the conditions of the laboratory experiments (Brakstad et al., 2018). Other studies have focused mainly on the NSA, NDMA that has been of concern in drinking water in other contexts (Nawrocki & Andrzejewski, 2011). One *in-situ* study found NDMA to biodegrade in a groundwater system (half-life of 70 days, Zhou et al. (2009)). While this has been supported by several laboratory experiments (both aerobic and anaerobic), there are also laboratory experiments documenting the opposite; not finding NDMA to biodegrade under the duration of their experiments, up to 100 days (summarised in Kumar et al., 2023; Nawrocki & Andrzejewski, 2011). The biodegradability of a molecule is challenging to predict since the process will depend on the structure of the compound, various environmental parameters (e.g., nutrient composition and oxygen levels), and on the types and numbers of the microorganisms present (see e.g., Meckenstock et al., 2015; Providenti et al., 1993). For NAs associated with explosives, reliable studies are available. While these substances have the same nitro-functional group (-NO₂), they are typically of larger size and with cyclic/aromatic structures. Several studies document biodegradation of these explosive-related NAs, both under aerobic and anaerobic conditions, though with long *in-situ* measured groundwater decay (see e.g. Bernstein et al. (2010)). Interestingly, some studies suggest the degradation to start by cleavage of the nitro-functional group (as summarised by, Deepak et al., 2015; Ju & Parales, 2010; Kalderis et al., 2011). This can indicate a “universal” NA-biodegradation pathway potentially also applicable to the NAs associated with CO₂ capture. See Appendix B for details.

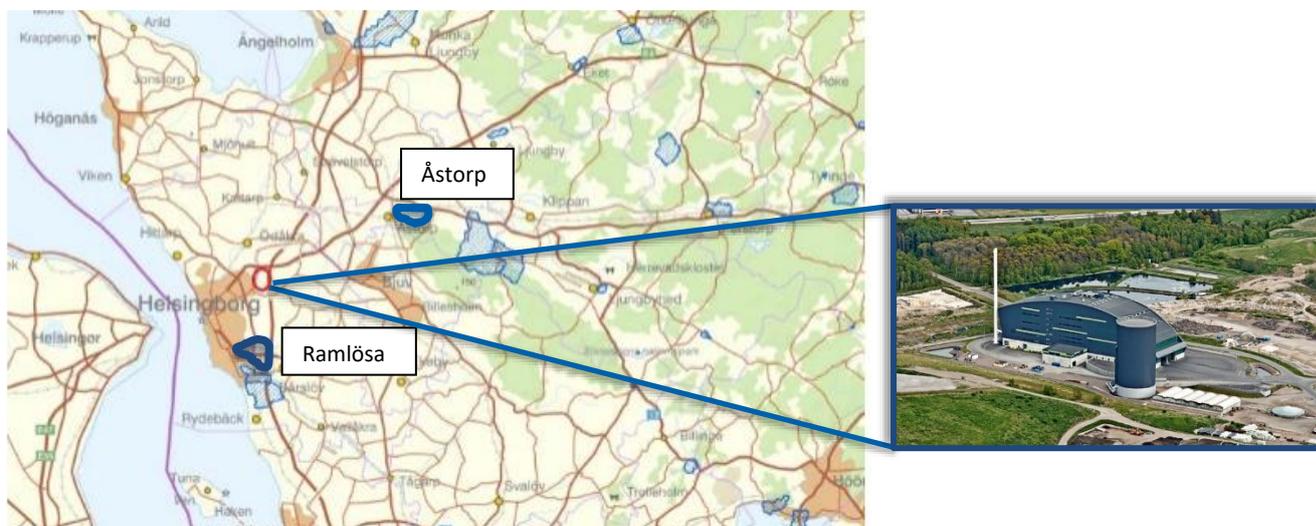


Figure 1: Map showing the location of the Filborna EfW plant (red circle) in relation to the water protection areas (blue shading). The two areas in this study are given a thick blue outline. Edited from (Borgnes & Price, 2023). Photo: Öresundskraft.

Aim of the study:

The aim of this assessment was to simulate future concentrations of NSAs and NAs in two groundwater basins near the Filborna EfW plant at where CO₂ capture is underway. The two selected basins were Ramlösa Hälsobrunn and Åstorp. The simulations were computed using the catchment model INCA-contaminants (hereafter: INCA-Tox), which incorporates the various key influencing biogeochemical processes discussed above and allows for assessing potential accumulation with time.

¹ For full molecular names and CAS numbers, see Appendix B.

2 Materials and methods

2.1 Catchment model

The catchment model, INCA-Tox (Nizzetto et al., 2016) was used to simulate the NSA and NA transport in the catchment and to predict future levels in the two groundwater basins. It is a high-resolution and dynamic catchment model that builds on the hydrology model PERSiST (Futter et al., 2014). In general, contaminants that enter the soil through atmospheric deposition are dynamically partitioned between solid and aqueous phases in the soil, groundwater, and river, and transported along the various water flow paths. Degradation of contaminants in all phases and compartments is computed. The model is fed with site-specific numeric information, including catchment characteristics and climatic conditions to establish a site-specific scenario. Then, the concentration of the contaminants at a selected place in the catchment (here: groundwater) can be estimated, and future predictions can be made.

The underlying hydrology in the PERSiST model drives the contaminant transport in INCA-Tox. This model has an upper soil compartment and a groundwater compartment. These are modelled as linear reservoirs, meaning that they have a maximum retention volume. Water in excess of the retention volume will flow to e.g., a river at some constant given rate. This means that the contaminants in the INCA-Tox model are completely mixed within each of the two reservoirs. In reality, the groundwater may consist of several layers that are not well mixed, the consequence of which we discuss below. Thus, this approach will provide a conservative estimate of contaminant levels in comparison to the reality (*i.e.*, lower).

While PERSiST does not describe advanced groundwater dynamics like designated groundwater models such as the Modular three-dimensional finite-difference ground-water flow model – MODFLOW (Yager, 2020), it allows for coupling to the INCA-Tox contaminant module, which sophisticatedly incorporates the various key influential biogeochemical catchment processes described above in the introduction. The model is not dependent on detailed geological profile data. The groundwater reservoir residence time, T is defined by:

$$T = V/Q,$$

where V is the volume and Q is the average flow of water into- and out of the reservoir.

Finally, the model allows for an advanced uncertainty analysis to provide information on which of the processes are the most influential to the results. This is an important tool in setting the uncertainty range of the results, similar to the traditional “best case” and “worst case” model conditions.

The model itself (but not any of the data used for this report) is open source as part of the Mobius framework, and the specific implementation can be viewed at GitHub:

<https://github.com/NIVANorge/Mobius/blob/master/Modules/INCA/Persist.h>

<https://github.com/NIVANorge/Mobius/blob/master/Modules/INCA/INCA-Tox.h>

2.2 Site description

The two groundwater basins, Ramlösa Hälsobrunn and Åstorp, were selected for the catchment modelling since these were found, from the atmospheric dispersion and deposition modelling, to receive the highest loadings of NSA and NA (Borgnes & Price, 2023). See Table 1 for details of the two sites and Appendix A for water chemistry data. Figure 2 illustrates the bedrock aquifers.

Table 1: General descriptive parameters of the two studied groundwater basins.

Parameter	Ramlösa hälsobrunn	Åstorp
ID	NVR-ID 2012279	NVR-ID 2012368
Residence time	> 65 years	Unknown*
Bedrock	Jurassic sandstone	Siltstones, sandstones, claystones, and clay
Hydraulic conductivity	5.08 – 5.71 m/s	4.40 – 7.74 m/s

*based on the limited available knowledge, set to 5-20 years as a worst-case scenario.

The groundwater reservoir in the Ramlösa area is in sedimentary rock marked with a fractured and porous bedrock (Gustafsson, 1999). See Figure 2. The water sold by the Ramlösa carbonated water company is described by Gustafsson et al. (2005) to be abstracted from “a sandstone at greater depth”. The age of the water from the Ramlösa Hälsobrunn aquifer, according to the information available on the company’s webpage is 70 years (<https://ramlosa.se/vart-vatten>). This is corroborated by an age dating carried out using chlorofluorocarbons, which estimated the age of the water to be 65 years or more (GEUS, 2007, as cited in Ekström (2009)).

Groundwater abstracted by the Åstorp municipality is from aquifers in bedrock and soil layers. The major sedimentary bedrock in the area is part of the Ljungbyhed 1 a & b groundwater system (Gustafsson, 2011), which is a confined aquifer of thickness between 250 and 500 m and with an area of 34 km². The soil aquifer is part of the Kvidinge - Klintarp - Ljungbyhed groundwater reservoir system for which the thickness ranges between 20 and 40 m (Gustafsson, 2010). Gustafsson (2011) describes that the groundwater resource in the area shows great variability due to variations in the composition of the aquifers which cover siltstones, sandstones, clay stones, and clay. Unfortunately, it has not been possible to find studies that describe the age of the groundwater in the soil and bedrock aquifers of Åstorp. Assessment of age distribution of groundwaters of 25 public supply wells within the Scania county was conducted by Åkesson et al. (2015) with the use of multiple tracers. They estimate that the mean age for waters from unconfined sedimentary aquifers to be less than 30 years. To be conservative we have assumed an age between 5 and 20 years for Åstorp municipality’s groundwater resources.

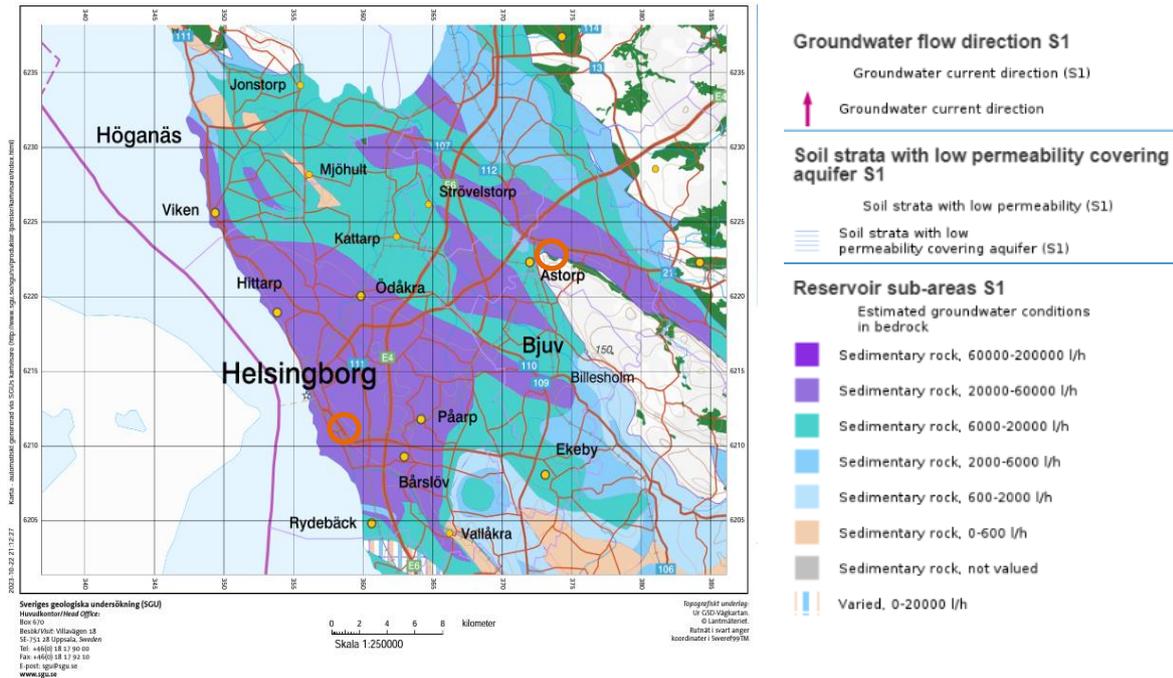


Figure 2: Overview of the sedimentary aquifers in the study area showing Ramlösa Hälsobrunn (close to Helsingborg) to be located in the purple region, indicating sedimentary rock, and Åstorp to be located in the green and white areas. Source: (Gustafsson, 1999).

2.2.1 Catchment hydrology and model parameterisation

The hydrology in the model (PERSiST) was setup for the sub-catchment outlined in Figure 3 which covers the Ramlösa recharge zone. The model used daily temporal resolution and covered the years from 2010 to 2022. Table 2 presents values of selected model parameters. The catchment has previously been modelled using the hydrology model HYPE (Andersson & Nisell, 2019; Lindström et al., 2010). Thus, this allowed our model to be validated by comparing results to the previous study (Lindström et al., 2010). The data used was available online from the Swedish Agency for Marine and Water Management (SMHI) (<https://vattenwebb.smhi.se/modelarea/>).

For both sites, Ramlösa and Åstorp, the same upper layer hydrology was applied. This can be justified based on their proximity in space and that there is no indication of the surface hydrology being significantly different between the two sites. Also in confirmation, the existing HYPE model setup was almost identical for these two locations (Lindström et al., 2010). Note that the groundwater retention time was separately varied at the two sites in the scenarios described below.

The validity of the hydrology parameterization was assessed in two different ways. First, our simulated hydrology was compared to that from the previous study using the HYPE model. A strong correlation was found between the two model outputs, which is illustrated in Figure 4 for water discharge. Moreover, a Nash-Sutcliffe efficiency coefficient of 0.81 was achieved. This ensures a realistic simulation of the hydrology of the main flow paths, the residence time in the upper compartment of the model, and the evapotranspiration. Second, our INCA-Tox model output for water fullness in the Ramlösa basin was compared to the output from a SGU (Geological Survey of Sweden) simulation using a different model (<https://www.sgu.se/grundvatten/grundvattennivaer/berakningsmodell/>). There was a strong agreement for the timing of the recharge and depletion of the water in the basin (Figure 5).

Note that the groundwater basin in our model may not overlap exactly with the one modelled by SGU, so this figure mostly shows that the timings of recharge and low levels is correct. Note also that the degree of water fullness is a metric used to estimate the status of an aquifer compared to its minimum acceptable water level. A degree of water fullness of 0% does not mean that the aquifer is empty, but rather that there is too little water for sustainable water extraction. The actual volume of the aquifer is much greater. Thus, deviations in the absolute degree of water fullness will not have a large impact on contaminant concentrations in the basin because of the large available volume of water.

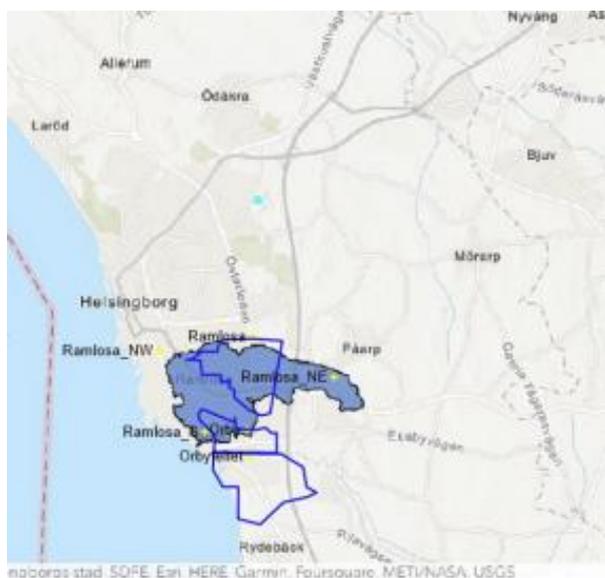


Figure 3: Map showing the area of the Råån catchment used to calibrate the model (blue shading), and the location of the water protection areas (blue lines). Edited from: (Borgnes & Price, 2023).

Table 2: Calibrated PERSiST parameters governing the water transport.

Name	Unit	Value
Baseflow index	1	0.1
Soil water time constant	days	7
Groundwater retention time	years	Ramlösa: 65, Åstorp: 5-20
Degree-day evapotranspiration	$mm\ ^\circ C^{-1}\ day^{-1}$	0.19
Growing degree threshold	$^\circ C$	2.81

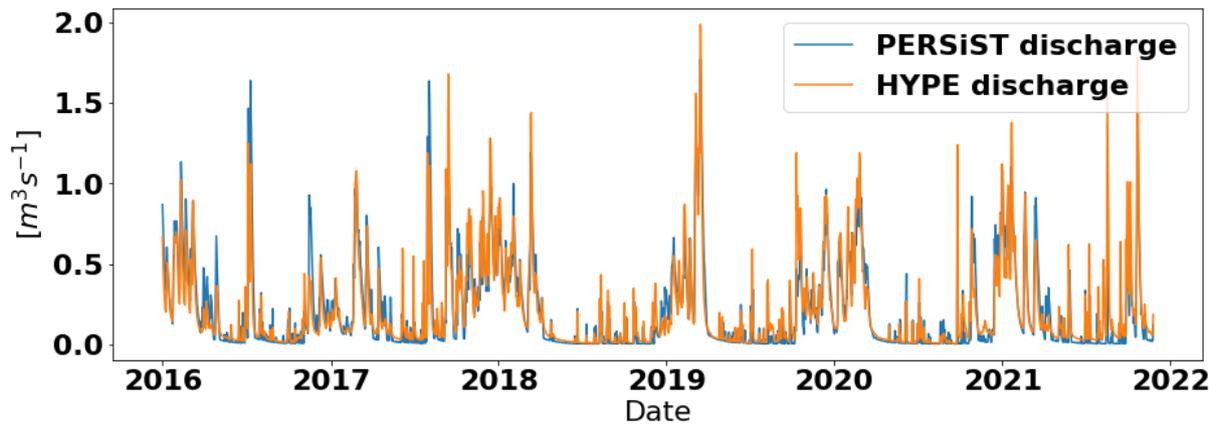


Figure 4: Comparison of the discharge ($m^3 s^{-1}$) over time using our model (blue) and the HYPE model (orange), for the sub catchment of Råån.

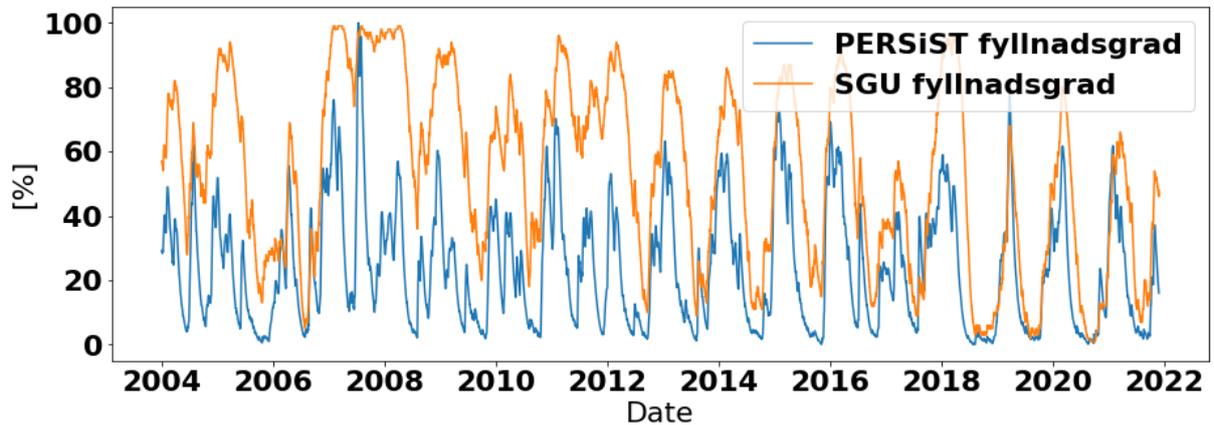


Figure 5: Comparison of the water fullness (% , sv: fyllningsgrad) our model (blue) and SGU model (orange) for the groundwater basin at Ramlösa. The SGU modeled data is for “fyllningsgrad stora magasin” at site 52054, which covers southern Helsingborg and Ramlösa.

2.2.2 Climate

Table 3 lists key climatic parameter values that were used to describe the two sites Ramlösa and Åstorp. Air temperature and precipitation (P) data, spanning 1995-08-01 to 2023-03-01, was downloaded from the SHMI open database (<https://www.smhi.se/data/meteorologi/ladda-ner-meteorologiska-observationer>). The data was selected from the station Helsingborg A (station number 62040). The data was repeated by concatenating the values from 1996-01-01 to 2022-12-31 many times after one another to create an artificial precipitation and temperature scenario running until 2103. Other parameter values were taken from the HYPE model setup described above. The SHMI daily precipitation data had a lower average annual precipitation for the extracted period than what was reported in the HYPE model setup, but we achieved the same effective precipitation (P - E) where P is precipitation and E is evapotranspiration.

Table 3: Summary of climatic data used at both two study sites.

Variable	Value and unit	Source
Annual precipitation (P)	804 mm	HYPE model setup
Annual evapotranspiration (E)	519 mm	HYPE model
Annual mean air temperature	8.81 °C	SHMI database.
Annual mean soil temperature	7.86 °C	Modeled in INCA-Tox.

2.3 Atmospheric deposition rates

Data of NSA and NA atmospheric deposition rates were made available by Norsk Energi, in cooperation with Cambridge Environmental Research Consultants (CERC) (Borgnes & Price, 2023). In brief, the data was computed using an atmospheric dispersion and deposition model (ADMS 5 with amine chemistry module). The emission data was based on measurements from the pilot CO₂ capture plant at an EfW plant in Norway (Hafslund Oslo Celsio) and adapted to a worst-case amine solvent type, with regards to NSA and NA formation. Deposition data was used from the year 2021 that provided worst-case conditions for wind. The NSAs and NAs were treated as two generic compound groups. The grid resolution was 100 m and the temporal resolution hourly. See Table 4 for the sum of the dry and wet deposition of NSAs and NAs. For more details on the atmospheric dispersion and deposition model, and on operational conditions at the Filborna EfW plant, see Borgnes and Price (2023).

When constructing the model inputs, the deposition rates for 2021 was repeated for 118 years. The deposition rates were aggregated from hourly to daily values to fit the INCA-Tox model. Note that by using meteorological-dependent data that represents one year only, the expected natural year-to-year variation is not taken into consideration. This will apply to e.g. the distance and direction from the plant where the NSAs and NAs will be deposited.

Table 4: Annual averages of the daily dry and wet deposition rates ($ng\ m^{-2}\ day^{-1}$) of NSAs and NAs (Borgnes & Price, 2023).

Year	Ramlösa		Åstorp	
	Nitrosamines (NSAs)	Nitramines (NAs)	Nitrosamines (NSAs)	Nitramines (NAs)
2021	2.82	11.52	0.54	4.64

2.4 Molecular physiochemical properties

The values for key physiochemical parameters of the two generic groups of NSAs and NAs are listed in Table 5. The values are averages of some of the most studied NSAs (N-nitrosomonoethanolamine) and NAs (N-nitromethylamine, Dimethylnitramine, N-nitromonoethanolamine) as well as a few censored NSAs and NAs that was also included in the environmental assessment at the Norwegian EfW plant (Norling et al., 2022). Information on these censored compounds was provided by prof. emer. Claus J. Nielsen (person. comm.).

Table 5: Selected parameters for properties of nitrosamines (NSAs) and nitramines (NAs).

Parameter name	Symbol	Unit	Value	
			Nitrosamine (NSA)	Nitramine (NA)
Molar mass*	Mm	g mol ⁻¹	74.1	90.7
Molecular volume**	Mv	cm ³ mol ⁻¹	56.5	90.7
Henry's constant at 25 °C	H	Pa m ³ mol ⁻¹	0.104	0.081
Log10 Octanol-water partitioning coefficient*	Log ₁₀ K _{OW}		-0.7	-0.9

*Calculated using EPISUITE software.

**Assuming a density of 1 and 1.31 for the NAs and NSAs, respectively (prof. emer. Claus J. Nielsen)

***Typical values for semi-volatile substances (Schenker et al., 2005; Shen and Wania, 2005).

2.5 Aqueous phase removal processes

Aqueous phase removal processes cover biogeochemical processes that remove NSAs and/or NAs from the aqueous phase, either by transfer to another medium (e.g., soil or atmosphere) or by transforming the molecule into another (e.g., biodegradation or photodegradation). The result is a lowered concentration of NSAs and/or NAs in the aqueous phase. Here follows a presentation of key processes included, and an evaluation of the parameter values selected. Most focus is devoted to biodegradation which was found both to be both influential and uncertain.

Abiotic hydrolysis has been found not to be of importance for the relevant NSAs and NAs (Sørensen et al., 2015). Note that NSA volatilisation from soil water to air was turned off in the model due to a lack of knowledge on how to parametrize it. Moreover, while photodegradation is an important depletion pathway for NSAs in exposed surface water (e.g., lakes), it is not considered here since it does not occur once the NSAs have entered the soil water. Surface water is not considered in this study.

2.5.1 Biodegradation

The biodegradation rate (R_{bio} ; day⁻¹) was formulated as follows, for both NSAs and NAs, in both catchment compartments, and using a common Q_{10} -type response to temperature, defined as:

$$R_{bio} = K_{bio} Q_{10}^{\frac{(T_{water}-T_0)}{10}}$$

where K_{bio} is the biodegradation rate at temperature T_0 (day⁻¹), q_{10} is the temperature adjustment coefficient to a 10°C change in temperature (unitless), and T_{water} is the water temperature (°C) in the given compartment. In practice, we computed K_{bio} from a half-life (hl) via $K_{bio} = \ln(2)/hl$. The parameter values are summarised in Table 6.

In the model, different parameter values were used for NSA and NA half-life between the upper soil-water layer and in the groundwater layer. In the upper layer, a half-life of 2 years was selected. This

was considered to be conservative, based on the findings by Brakstad et al. (2018). Under aerobic and anaerobic lake-water conditions, a half-life of ~30 days was reported for a few relevant NSAs and NAs. However, in the study, some of the NSAs and NAs were found not to biodegrade during the duration of the experiments (56 days). This likely resulted from the biodegradation of these compounds taking longer than the duration of the experiments and/or that the experimental conditions were not favourable (Meckenstock et al., 2015). In any case, it should be noted that there is uncertainty related to this parameter value.

In the groundwater layer of the model, the biodegradation half-life was very uncertain due to limited studies found for groundwater conditions. For the one NSA, NDMA, Zhou et al. (2009) found *in-situ* groundwater half-life to be 70 days in a basin in Los Angeles County, California, USA. However, a similar biodegradation rate has not always been found in studies of NDMA by laboratory experiments. The reason for the conflicting results is, again, most likely differences in key conditional parameters. It is challenging to translate results from a laboratory biodegradation experiment to real groundwater conditions due to the heterogeneity of a groundwater basin (Grösbacher et al., 2018). In fact, factors controlling biodegradation is in a general sense a large open scientific question. With the words of Meckenstock et al. (2015), "...it is totally unclear how microbial metabolism is regulated in the environment."

Despite this, a few general points can be made, mainly based on (Meckenstock et al., 2015, and references therein). A groundwater basin is inhabited by a range of different types of bacteria. The bacteria are dominantly attached to surfaces rather than freely dissolved in the water phase. Thus, while the bacterial cell count for the groundwater was reportedly low (Appendix A, Table A.1), this does not mean that the basin is sterile, and that biodegradation cannot occur. Further, biodegradation is typically a process for the bacteria to respire, and the presence of other electron donors (or acceptors) are needed. Table A.1 shows the presence of Mn, Fe, and SO₄. The oxygen concentration is not reported, but the overall water chemistry indicates that it is low. For very recalcitrant molecules, anaerobic conditions are often required. A low oxygen level in the water may facilitate for the development of anaerobic conditions, such as in micropores.

While the "right types" of bacteria may be present in the groundwater basin, the bacteria may be dormant and require time to establish sufficient cell numbers. The doubling time for bacteria in groundwaters may be months to years. Studies of other types of contaminants, anticipated to be less biodegradable based on molecular structure, have found groundwater half-lives to exceed 100 years, see e.g., Bernstein et al. (2010). However, once the degraders have been established, in response to the contaminant, the biomass may persist for months and perhaps even years after the source of contamination has disappeared (Meckenstock et al., 2015). This is of importance to CO₂ capture, from which a low level of NSAs and NAs are expected to prevail over time rather than constituting a one-time point release. Other important factors for groundwater biodegradation are the flow velocity and the concentration of the contaminant, which can have different effects on the outcome (Grösbacher et al., 2018; Nawrocki & Andrzejewski, 2011)

Thus, based on available literature, our educated guess is that the NSAs and NAs are likely to biodegrade under these groundwater conditions. But the time needed for the rates to have a significant impact on the water concentration is very uncertain. For the groundwater layer of the model, the biodegradation half-life was set to 10 years for a worst-case scenario and with simulations varied down to 2 years.

Table 6: Parameters used in the biodegradation removal processes.

Process	Symbol	Value	Unit	Note
Biodegradation	K_{bio} (at T_0) gw	0.00018-0.00095	day^{-1}	*
	K_{bio} (at T_0) soil	0.00095	day^{-1}	**
	Q_{10}	1.63	1	***
	T_0	7.86	$^{\circ}C$	****

* This corresponds to half-lives of 2-10 years.

**This corresponds to a half-life of 2 years.

*** Equiv. to 5% change per $1^{\circ}C$.

**** This was set to the annual mean modelled soil temperature at the site to make comparisons with the control calculations easier.

2.5.2 Soil sorption

In the upper soil layer, the contaminants partition between water and soil organic carbon with the following fraction

$$q = K_{oc}c$$

where q is the concentration of contaminants in the soil organic carbon (ng/kg OC), and c is the concentration in water (ng/l). K_{oc} is derived from K_{ow} (see Table 5). The formula is described in the INCA-Tox supplementary material in Nizzetto et al. (2016). The amount of contaminant found to sorb to the soil carbon is also subject to biodegradation, and thereby allows additional contaminant molecules to sorb to the soil.

In the groundwater basin, potential influence from NSA and NA sorption to bedrock was not included. Given the high solubility of NSAs and NAs in water, and the low soil sorption rates found in the literature (Gundersen et al., 2017; Gunnison et al., 2000), loss of NSAs and NAs from the aqueous phase due to sorption to non-organic solids was anticipated to represent a negligible fraction.

2.6 Simulated scenarios

The study was conducted at daily time steps for 118 years to assess the potential accumulation of the NSAs and NAs with time. It is not certain that the plant will be active for 118 years, so such a long contamination could be considered a worst-case scenario. It should also be noted that we do not include climate effects in our modeled scenarios. Since precipitation and temperatures are likely to increase (Eklund et al., 2015), the likely impact of that would be faster replenishment of the groundwater resulting in lower contaminant concentrations. While the impact on degradation rates would be uncertain, they are not likely to be large enough to change the main conclusion of the results.

The model was run for various combinations of residence time, T and biodegradation half-life, hl . This was due to the following two factors:

1. The biodegradation in the groundwater (apart from the deposition rates) is the process that is the most impactful on modeled concentrations in the water. The impact of this process is governed by the amount of time the water stays in the basin and the speed at which the degradation occurs.
2. The values of these two parameters are highly uncertain due to lack of open knowledge about water residence time or well size (at least for Åstorp) and biodegradation rates of NAs and NSAs in groundwater.

The residence time at Ramlösa was set to 65 years, which was considered worst case for that location, while the residence time at Åstorp was set to range between 5 and 20 years (see discussion in section 2.2). The biodegradation half-life in the groundwater was set to range between 2 and 10 years (see discussion in section 2.5.1). For reference, simulations were also computed with biodegradation set to zero.

2.7 Control calculations

Two simplified control calculations, called the Vollenweider equation and “A moving parcel of water”, were set up to check that the INCA-Tox model produced sensible results. In both control calculations the two following simplifications were made: The groundwater recharge Q was assumed to be given by $Q = A(P - E)$, where A is the catchment area, P is precipitation and E is evapotranspiration. Second, the recharge is equal to the sum of runoff and extraction so that the groundwater volume V will stay constant. The concentration c_0 of contaminants in groundwater recharge is $c_0 = Af/Q$, where f is the total (dry+wet) contaminant deposition per unit area. Contrary, in the INCA-Tox setup, Q , V and c_0 are dynamically computed by the model processes.

2.7.1 Control 1: The Vollenweider equation

Assuming the groundwater basin is always completely mixed (which is the case in INCA-Tox) and all rates are constant, the mass of contaminants in the groundwater can be described by the following differential equation:

$$\frac{dm}{dt} = Qc_0 - Q\frac{m}{V} - K_{bio}m,$$

where m is the mass of contaminants in the reservoir, c_0 the contaminant concentration in the water as it enters the reservoir, and $K_{bio} = \ln(2)/hl$ is the biodegradation rate at the annual mean soil temperature. Assuming $V = QT$, where T is the mean residence time, one can show that this system after sufficient time approaches an equilibrium which can be described by:

$$c = \frac{m}{V} = \frac{c_0}{1 + K_{bio}T}$$

This is called the *Vollenweider* equation (Vollenweider, 1975), and it will give the concentration in the extracted water after the system has reached equilibrium assuming constant Q and c_0 .

2.7.2 Control 2: A moving parcel of water

With slightly different dynamics, if we assume a *parcel* of water that travels downward in the reservoir without mixing until it is extracted, then the concentration of contaminants in that parcel obeys the following equation:

$$\frac{dc}{dt} = -K_{bio}c$$

So, at the time of extraction the concentration in the parcel will be:

$$c(T) = c_0 e^{-K_{bio}T}$$

where T is now the amount of time the parcel spends in the reservoir (travel time rather than residence time).

3 Results and discussions

3.1 Future levels of NSA and NA in the groundwater basins in comparison to the safety limit

Modelled groundwater concentrations for the sum of NSAs and NAs over time are shown in Figures 6 and 7 for Ramlösa Hälsobrunn and Åstorp, respectively. The time extends for more than 100 years, and the NSA and NA concentration was assumed to be zero at the start. It should be noted that it is unknown what the background concentrations of NSAs and NAs are.

The blue line in Figure 6 depicts NSA and NA concentrations considering a residence time of 65 years and a biodegradation half-life of 10 years. There is a relatively rapid increase during the first ~25 years of operation of the CO₂ capture plant before the level stabilises at around 2 ng L⁻¹. This is well below the recommended safety limit for drinking water (4 ng L⁻¹, Låg et al. (2011)). The initial increase reflects the time needed for the system to equilibrate to the new input. While the water residence time has been verified (<https://ramlosa.se/vart-vatten>; GEUS, 2007, as cited in Ekström (2009)), the magnitude of the biodegradation half-life was more uncertain. With a shorter half-life, between 2 to 10 years, the concentration of NSA and NA is reduced (Figure 6, grey shaded area). On the contrary, for the NSA and NA concentration to reach above the safety limit, the half-life would need to be more than 23 years (data not shown).

At Åstorp, the future scenario of NSA and NA levels in the groundwater runs a little different (Figure 7). The main reason for this is that the residence time is expected to be lower, and that the exact value for this parameter is unknown. The initial increase in NSA and NA is steeper with the shorter residence time and stabilises after ~10 years. Due to the uncertainty related both to the water residence time at Åstorp and the biodegradation half-life of the NSAs and NAs, the range of possible concentrations depicted by the grey shaded area range between 1.0 and 3.2 ng L⁻¹. This means that even when using the here anticipated worst-case settings for the two parameters of water residence time (T = 5 years) and biodegradation half-life (hl = 10 years), the concentration remains below the recommended drinking water limit. It is important to point out that high uncertainty is still associated with the worst case setting of biodegradation half-life. The half-life would need to be longer than 25 years for the concentrations to exceed the safety limit.

The studied basin at Åstorp is shallower than at Ramlösa. This could indicate a faster biodegradation rate at Åstorp, in comparison to Ramlösa. However, the magnitude of this difference is not possible to estimate with current knowledge. With the half-life fixed at 10 years, the residence time must be above 16 years for the concentration levels to be below the safety limit (data not shown).

At both sites, the groundwater concentration is expected to be dominated by NAs. This is a reflection of the deposition rates which showed 80-90% NAs by mass (Table 4, Borgnes and Price (2023)).

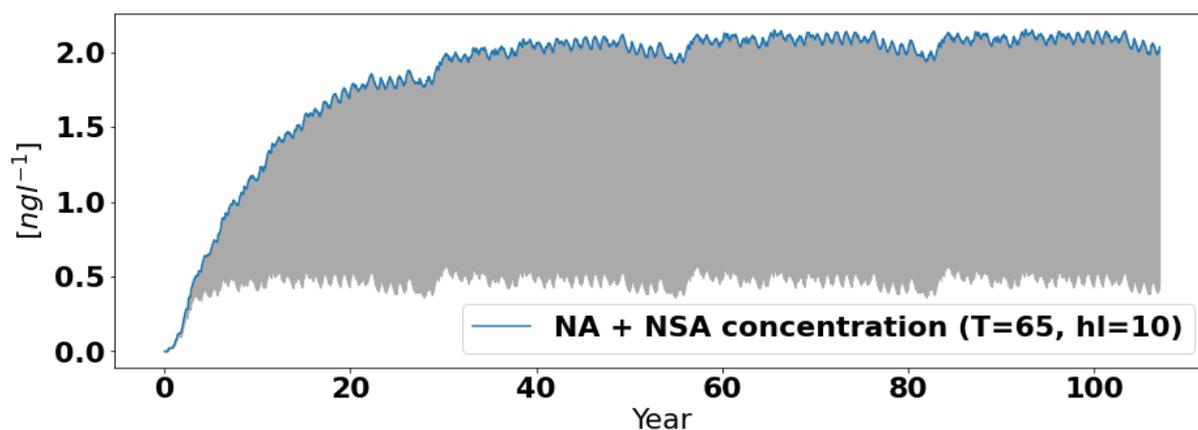


Figure 6: Modelled concentrations for the sum of NSAs and Nas in the Ramlösa groundwater basin over time. The blue line signifies the concentration with the configuration of groundwater residence time (T) at 65 years and with a groundwater half-life (hl) of 10 years. The grey area shows the range of concentrations within the configurations T = 65 years, and with hl = 2 to 10 years.

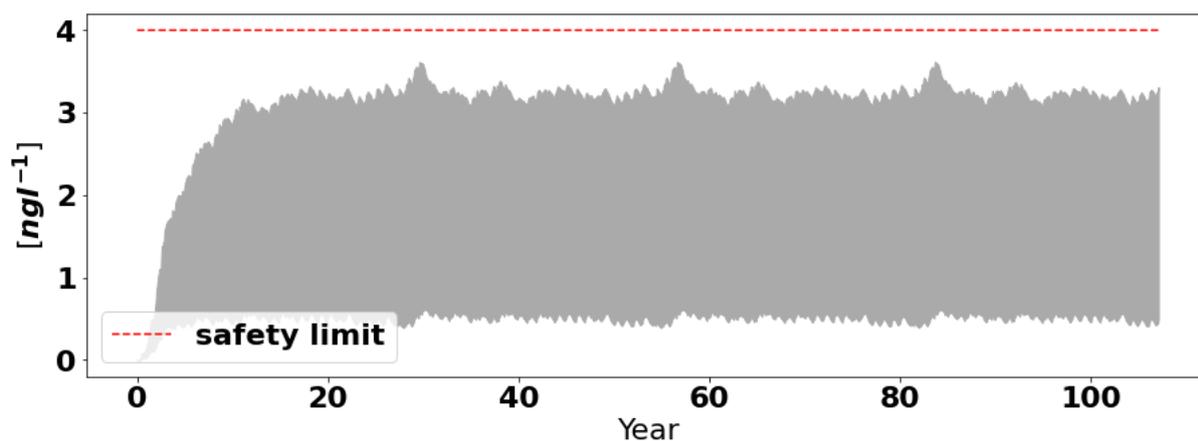


Figure 7: Modelled concentrations for the sum of NSAs and Nas in the Åstorp groundwater basin over time. The grey area shows the range of concentrations within the configurations T = 5 to 20 years, and with hl = 2 to 10 years. The red dotted line indicates the NIPH recommended drinking water safety limit.

3.2 The importance of biodegradation for groundwater NSA and NA levels

The process of biodegradation was found to have a large impact on the resulting NSA and NA concentrations, and at the same time being associated with a high uncertainty. To demonstrate the effect of biodegradation, Figure 8 shows the evolution of NSA and NA levels in the groundwater basin at Ramlösa over time when the half-life in the groundwater layer is set to zero (biodegradation at the half-life in the soil-layer is set to 2 years). The concentration exceeds the safety limit after about 25 years of running the CO₂ capture plant. Further, modelled concentration will rise to 10 ng L⁻¹ over a 118-year period, and at this point the maximum level has not even been reached. In the even more unlikely scenario of having also no removal processes taking place in the soil layer, the concentrations will reach 19 ng L⁻¹ after a number of years (data not shown). However, these are considered very unlikely scenarios on the background of the discussion in section 2.5.1. In brief, groundwater basins are inhabited by a range of different types of bacteria; some of the NSAs and NAs have been found to biodegrade under (anoxic and oxic) laboratory experiments; one of the NSAs has been proven to *in-situ* biodegrade in a groundwater basin; and the water chemistry from Ramlösa and Åstorp give indication of possible biodegradation.

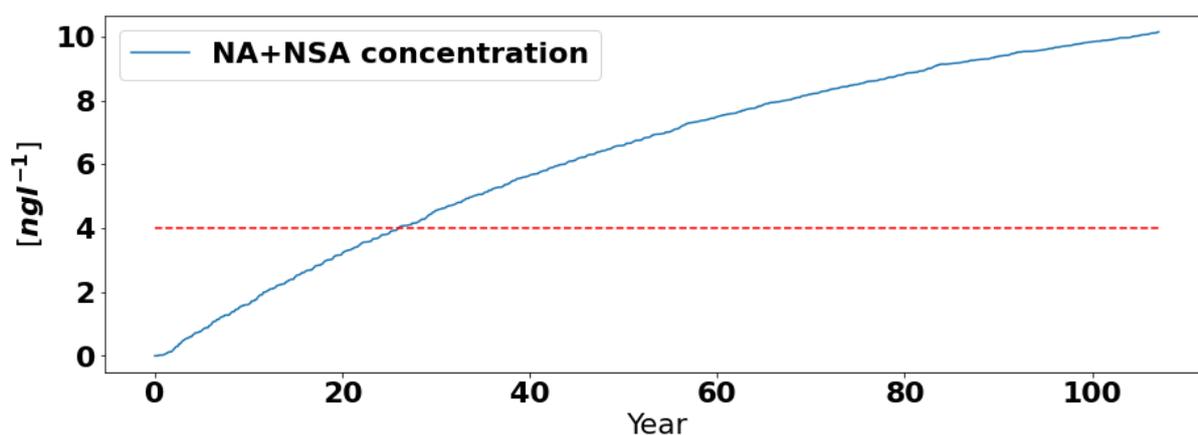


Figure 8: Modelled concentrations for the sum of NSAs and NAs in the Ramlösa groundwater basin over time with no biodegradation in the groundwater. The blue line signifies the concentration with the configuration of residence time (T) at 65 years and with no biodegradation taking place. This is considered a highly unlikely scenario. The red dotted line shows the NIPH recommended drinking water safety limit.

3.3 Impacts from varying the residence time and half-lives

Two different control calculations were run to validate the model output. Table 7 compares the NSA and NA concentrations computed with the two different types of control calculations and INCA-Tox, and by using different combinations of water residence time and biodegradation half-life. Results are presented both for Ramlösa and for Åstorp.

Overall, there is sufficient agreement between the output from the INCA-Tox model and the two control calculation methods. The concentrations are lower in the output from INCA-Tox compared to that from the Vollenweider computations. This is mainly because in INCA-Tox there is also sorption and degradation of the contaminants to the soil layer included. In comparison to the output from 'Parcel' the INCA-Tox model output is either lower or higher, depending on the parameter values of retention time and half-life. In 'Parcel' nothing was removed in the upper soil layer, so if biodegradation is low in the groundwater, 'Parcel' also shows a higher concentration than INCA-Tox, which may be unrealistic since we expect some removal in the soil layer. 'Parcel' can be said to have a more realistic description of the movement of water in the groundwater layer, assuming that the extracted groundwater is old and not completely mixed with the newly infiltrated water. In INCA-Tox, complete mixing of the entire groundwater basin is assumed (representing a worst case). Thus, the reality may be somewhere between INCA-Tox and 'Parcel' in the cases where 'Parcel' is lower than INCA-Tox.

Scenarios considered to be more likely, based on the available documentation, are marked in grey. Note that for Åstorp there are several more likely scenarios than for Ramlösa. This results from the larger uncertainty associated with information describing the groundwater at Åstorp.

Table 7: Analytical (control calculation) and simulated concentrations of NAs+NSAs in extracted water ($ng\ l^{-1}$) after a long time (depending on computation type) of steady deposition. (T=residence time (years), hl = half-life (years)). The INCA-Tox concentration is not necessarily the equilibrium but is the average concentration in 118 years. Scenarios we consider more likely are highlighted.

T	hl	Ramlösa			Åstorp		
		Control 1 (Vollen.)	Control 2 (Parcel)	INCA-Tox	Control 1 (Vollen.)	Control 2 (Parcel)	INCA-Tox
5	2	7.1	3.4	4.0	2.6	1.2	1.4
5	5	11.4	9.7	6.9	4.1	3.5	2.4
5	10	14.4	13.7	9.1	5.2	5.0	3.2
5	∞	19.4	19.4	13.0	7.0	7.0	4.6
10	2	4.3	0.6	2.3	1.6	0.2	0.8
10	5	8.1	4.8	4.7	2.9	1.8	1.7
10	10	11.4	9.7	7.0	4.1	3.5	2.5
10	∞	19.4	19.4	12.9	7.0	7.0	4.6
20	2	2.4	0.0	1.3	0.9	0.0	0.5
20	5	5.1	1.2	2.9	1.9	0.4	1.0
20	10	8.1	4.8	4.8	2.9	1.8	1.7
20	∞	19.3	19.3	12.7	7.0	7.0	4.5
65	2	0.8	0.0	0.4	0.3	0.0	0.2
65	5	1.9	0.0	1.1	0.7	0.0	0.4
65	10	3.5	0.2	2.0	1.3	0.1	0.7
65	∞	19.3	19.3	10.1	7.0	7.0	3.6

4 Conclusion and outlook

An advanced catchment model was used to simulate water concentrations of NSAs and NAs in two groundwater basins at Ramlösa Hälsobrunn and Åstorp, located near the planned CO₂ capture plant at the Filborna EfW plant. The model produced a good fit for the site-specific hydrological variables which indicated a high degree of site specificity of the simulations. Key biogeochemical processes were included in the model, among which the two parameters groundwater residence time and biodegradation half-life were identified as both influential and uncertain.

At Ramlösa Hälsobrunn, the NSA and NA concentration was found to increase during the first ~25 years of operation at the CO₂ capture plant, before stabilising at around 2 ng L⁻¹, which is below the recommended drinking water safety limit (4 ng L⁻¹). These results were obtained with the assumption that the NSA and NA biodegradation half-life is 10 years or less. With few studies assessing the biodegradability of relevant NSAs and NAs available in the literature, this parameter value is associated with a relatively high uncertainty. Pushing the extreme of the half-life, beyond what is here considered likely, the safety limit would be exceeded if the half-life was more than 22 years.

At Åstorp, the situation was less clear since the exact water residence time was not known but believed to be shorter than at Ramlösa. The ranges of likely values of water residence time and biodegradation half-lives suggest that the concentration at Åstorp will stabilise between 1.0 to 3.2 ng L⁻¹. This was computed using a water residence time between 5 and 20 years, and with the same biodegradation half-lives as for Ramlösa.

In conclusion, based on available literature and the herein presented model simulations, it is unlikely that the groundwater at Ramlösa Hälsobrunn will reach levels of NSAs and NAs that exceeds the safety limit. At Åstorp, even though it receives less deposition, the results have higher uncertainty because the age of the extracted water is lower and because the estimated concentrations come closer to the safety limit. Still, we estimate that they will remain below this limit.

It is important to note that in the entire chain of calculations, including the atmospheric dispersion and deposition model as well as the catchment model, worst case scenarios are applied to every uncertain parameter. For the catchment model used, the inherent assumption of the water being completely mixed adds up to this. In reality, the water extracted is old and is not mixed with newly infiltrated water. The use of a more sophisticated groundwater model describing the different depth layers of water and how they mix with one another can be valuable. The likely output from this is a lower NSA and NA concentration in the bottom layers. In addition, dating of the extracted water with environmental tracers (e.g., Åkesson et al. (2015)) can provide insights into the residence time at Åstorp and thereby reduce the uncertainty in the present modelling.

Future research studies should focus on producing NSA and NA biodegradation half-lives relatable to groundwater conditions, as well as acquiring a more certain estimate of the water residence time at the Åstorp groundwater basin.

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Appendix A.

Table A.1: Selected water chemistry parameters describing water from groundwater wells representing the two aquifers, Ramlösa Hälsobrunn and Årby. The analyses have been conducted by Eurofins Environment Sweden AB Lindköping and was made available by Helsingborg municipality (private communication).

Parameter	Unit	Örby (similar to Ramlösa)		Åstorp	
		Drinking water 1 (Stenbrogården)	Drinking water 2 (Raus 6)	Raw water, Åstorp	Raw water, Kvidinge
Date of sampling		2015-08-18	2015-08-12	2023-02-01	2023-02-28
Culturable microorganisms 22 C	Cfu/mL	<1	3	<1	<1
Slow growing microorganisms	Cfu/mL	19	120	<1	1
Special group of soil-bacteria that may cause odour of water (Actinomycetes)	Cfu/100mL	<1	< 1	<1	<1
Water temp at sampling	°C	9.5	9.2	9	9
Turbidity	FNU	4.5	3.5	5.2	0.72
pH		7.6	7.6	8.1	8.0
Alkalinity	Mg HCO ₃ /L	250	230	230	190
Conductivity	mS/m	55	47	54	47
Chloride	mg/L	26	23	40	25
Sulphate	mg/L	30	20	32	45
Fluorid	mg/L	0.23	0.29	1.0	0.27
COD-Mn	Mg O ₂ /L	0.88	0.70	0.70	0.56
TOC	mg/L	NA	NA	<2.0	<2.0
Ammonium-N	mg/L	0.16	0.14	0.24	0.015
Phosphate-P	mg/L	0.0090	0.0090	NA	
Nitrate-N	mg/L	< 0.10	< 0.10	<0.10	<0.10
Nitrite-N	mg/L	< 0.0020	< 0.0020	< 0.0020	0.0050
Sodium	mg/L	23	11	44	14
Potassium	mg/L	3.0	2.8	4.12	4.2
Calcium	mg/L	74	76	46	70
Iron	mg/L	0.75	0.54	1.5	0.15
Magnesium	mg/L	5.7	6.3	9.7	9.6
Mangan	mg/L	0.26	0.037	0.12	0.41
Aluminium	mg/L	< 0.010	< 0.010	0.0017	0.0013
Copper	mg/L	< 0.020	< 0.020	0.00052	0.00025

Appendix B.

Tables B.1 and B.2 lists NSA and NA biodegradation half-lives from studies available in the literature. Note that the list is not a complete literature review. Focus is on the CO₂ capture relevant NSAs and NAs, and on studies with conditions relevant to this study.

Table B.1: Summary of literature biodegradation half-lives for some relevant nitrosamines (NSAs).

Short name	Name	CAS	Half-life (days)	Sample type	Conditions	reference
NDELA	N-nitrosodiethanolamine	1113-54-7	32.2*	Lake-water	aerobic	(Brakstad et al., 2018)
NDMA	Nitrosodimethylamine	62-75-9	NA			
NPz	Nitrosopiperazine	5632-47-3	NA			
NDELA	N-nitrosodiethanolamine	1113-54-7	25.0*	Lake-water	anaerobic	(Brakstad et al., 2018)
NDMA	Nitrosodimethylamine	62-75-9	NA	Groundwater	In-situ	(Zhou et al., 2009)
NDMA	Nitrosodimethylamine	62-75-9	70			
NDMA	Nitrosodimethylamine	62-75-9	> 100			
NMOR	N-nitrosomorpholine			Groundwater	Anaerobic	(Patterson et al., 2010)

*Includes lag-phase.

Table B.2: Summary of literature biodegradation half-lives for some relevant nitramines (NAs).

Short name	Name	CAS	Half-life (days)	Sample type	Conditions	reference
DMNA	Dimethylnitramine	4164-28-7	NA	Lake-water	aerobic	(Brakstad et al., 2018)
MEA-NO ₂	Ethanolnitramine	74386-82-6	28.2*			
MNA	Methylnitramine	598-57-2	NA			
DENA	Diethylnitramine	7119-92-8	NA			
Pz-NO ₂	N-nitropiperazine	42499-41-2	NA			
AMP-NO ₂	1-methyl-2-(nitroamino)-1-propanol	1239666-60-4	35.1*	Lake-water	anaerobic	(Brakstad et al., 2018)
DMNA	Dimethylnitramine	4164-28-7	181*			
MEA-NO ₂	Ethanolnitramine	74386-82-6	14.1*			

*Includes lag-phase.



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