# Introduction

Fresh groundwater resources in coastal regions are a topic of study that may become increasingly important in the face of challenges of modern times: environmental, socio-economic, and geopolitical. Coastal regions are home to a significant share of humanity. In 2016, 44% of the world population was living within a 150km range of the coastline (J. Akrofi, 2016), where people largely rely on fresh groundwater resources, for domestic, industrial, and agricultural use (Delsman, 2015). In coastal areas, fresh groundwater resources are susceptible to degradation due to their proximity to saline seawater, high demands, land use change, climate change and sea level fluctuations (Werner et. al., 2013).

This study aims to assess and enhance state of the art groundwater modeling techniques for freshwater reservoirs in dunes. The coastline of the Netherlands is deemed a suitable study area for this aim, by virtue of extensive research and desirable study conditions (See section 1.2). The insights and analyses from this study may contribute to developing more efficient models used to increase the robustness and sustainability of drinking water resources in coastal areas globally.

## State of the Art

A prerequisite to sustainable management of coastal fresh groundwater reserves is an accurate description of their present-day distribution, which is difficult to obtain due to the sparse measurements at depth (Delsman, 2015). The coastline of the Netherlands may be an exception to this statement, as numerous studies have been conducted on its geohydrology, which provide a basis for further research. (Stuyfzand, 1993) conducted a hydrochemical facies analysis to identify the origins of over 2000 groundwater samples collected along the coastline; (Oude Essink, 2001) introduced the concept of a fresh-saline groundwater interface and discussed problems that arise in the Dutch coastline as a result of variable density flow, by using a numerical three-dimensional groundwater flow model; (Delsman, 2015) used a two-dimensional numerical model to perform a paleo-hydrological reconstruction, to investigate intrusion of saline groundwater from the sea over a longer timescale, throughout the Holocene.

Dunea manages drinking water supply from fresh groundwater reserves in the dunes of The Hague and seeks to increase their supply with 30% from 2021 to 2025 to account for future increases in demand, or deficits in precipitation due to climate change (Bootsma et al., 2021). In a preliminary study to investigate the feasibility of brackish groundwater as an additional source for producing drinking water, (Bootsma et.al., 2021) used a numerical three-dimensional state-of-the-art fresh-saline groundwater flow model to find that the extraction of brackish groundwater as a drinking water resource may be feasible, but that further research is necessary.

The state-of-the-art model’s applicability and reliability can be questioned, however, since it has only been calibrated on hydraulic head data (Bootsma et.al., 2021), potentially overseeing effects of variable density flow and thereby neglecting validation on groundwater salinity. Moreover, the model’s calculation times are impractical for use, exceeding 40 days for a simulation of 1000 years (REF) (not an uncommon simulation timescale for a geohydrological model), using powerful computing by Amazon Web Services.

The necessity for further research to increase the sustainability of drinking water in the dune area of the Netherlands and the questionable applicability of the state-of-the-art model’s results call for an assessment of conventional model validation techniques for drinking water management, that may contribute to efforts in coastal drinking water resource management globally.

Diagram

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Figure 1: Threats to coastal aquifers in the Netherlands. (Delsman, 2015)

## The coastal dunes of Meijendel-Berkheide as a study area

The densely populated coastal dunes and adjacent polders of the Western Netherlands suffer from all environmental evils of modern times. They are faced with a wide spectrum of natural variations and anthropogenic impacts, side by side as well as superimposed (Stuyfzand, 1993). Intrusion of saline groundwater, over extraction of freshwater resources, increase in demand due to growth, these are threats that coastal aquifers suffer in the Netherlands (see Figure 1).

The Netherlands has an elaborate history of water management. First accounts date back to 800AD, when drainage of coastal salt marches commenced (Delsman, 2015). Its rural landscape is characterized by polders, canals, and reclaimed lakes, initially drained using windmills. This pursuit dates to 1000AD (van der Ven, 1993), and is keeping water tables sufficiently low for agricultural use. Consequently, this drainage also resulted in compaction of soils due to oxidation of organic matter in peat soils, which were now exposed to air (Hoogland et. al., 2012).

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Figure 2: Study area of Meijendel-Berkheijde

In the area of Meijendel-Berkheijde, water management has a particular history, making it ideal to study the development of fresh-saline groundwater interactions over time, with human intervention. In the period of 1874 to 1955, excessive groundwater exfiltration caused significant desiccation and groundwater salinization in the dune area of Meijendel-Berkheide (Stuyfzand et al., 1993). To recharge the freshwater reserves, infiltration ponds were installed, and river water from the Rhine was pumped into the coastal aquifers since 1956. Since 1976 additional water from the Meuse River is pumped into the dune reserves to further enhance the reservoir’s recharge (see Figure 2).

Diagram

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Figure 3: Saline groundwater intrusion and overextraction in Meijendel-Berkheide, interpreted by (Stuyfzand, 1993). Cross section perpendicular to coastline, east-west. AM = Artificially infiltrated Meuse water, AR = Artificial Rhine, D = Dune freshwater.

Although it is found that long timescales are involved in establishing the current fresh-saline distribution in deltas (van Engelen, 2020) and salinity in the coastal groundwater of the Netherlands predominantly derives from sea water infiltration during Holocene marine transgressions (Post and Kooi, 2003), human intervention in coastal aquifers may disrupt this long timescale transience. As recognized by (Oude Essink, 2001), in areas where extensive human intervention (like extraction of groundwater) takes place, the anthropogenic influence on fresh-saline distributions may become primary, on a much smaller timescale. The geochemical analysis confirms that this is also the case in Meijendel-Berkheide (Stuyfzand, 1993).

Moreover, most data available are “snapshots” and provide little information on the long-term development of fresh-saline groundwater distributions. Modern techniques like the use of airborne electromagnetics to map groundwater salinity are on a relatively small timescale compared to the development of fresh-saline groundwater distributions. This lack of historical data causes model validation to be based on “snapshots”. Hydrochemical Facies Analyses (HyFA) like (Stuyfzand, 1993) may provide a contribution to model validation, as origin tracing provides insight in the “path” of water flow in the subsurface. The use of HyFA provides an opportunity to improve model validation techniques.

The coastal area of the Netherlands is judged as suitable for studying due to (a) an extensive amount of geohydrological studies and data obtained in the area for model validation (see section 1.1); (b) the HyFA providing insight in the path of groundwater flow in the area by (Stuyfzand, 1993), providing a research opportunity for fresh-saline groundwater model validation; (c) numerous studies with a successful numerical groundwater modeling approach in the area and (d) site specific human-induced conditions that disrupt the long timescales over which fresh-saline interfaces develop, consequently making the area preferable for modeling fresh-saline groundwater distributions efficiently, over a shorter period of time.

## Scope of Study

3D modeling techniques for fresh-saline groundwater interactions in coastal regions can be seen as the central concept of this study. Motivated by the conditions named in sections 1.1 and 1.2, the aim of this study is:

*To assess and improve efficient modeling practices and conventional model validation techniques for fresh-saline groundwater flow models used to study coastal drinking water resources.*

In this statement “*efficient modeling practices*” and “*model validation techniques*” require further specification. They are addressed in the following sub-objectives:

1. *Efficient modeling practices*: Increasing the efficiency of state-of-the-art groundwater flow model techniques while preserving accuracy.

2.1. Propose methods to increase efficiency

2.2. Review their effect on accuracy of model the model result

1. *Model validation techniques*: The suitability of Hydrochemical Facies Analyses (HyFA) for fresh-saline groundwater flow model validation, when investigating the hydrology of coastal fresh groundwater resources.

1.1. Assess conventional model validation techniques

1.2. Investigate suitability value of HyFA for model validation

## Report overview

Go through structure of paper.

# Modeling groundwater flow in coastal aquifers

Assessing conventional *efficient modeling practices* and *model validation techniques* through metamodeling is an iterative process that required addressing the underlying conceptual approach applied in this study. It is therefore necessary to first establish the theoretical foundation on which the model is constructed, this is done in section 2.1. Subsequently, the relevant modeling structure is explained in section 2.2. After this, the concept of regridding is introduced in section 2.3., which can be seen as one of the key methods in increasing modeling efficiency, potentially at the cost of efficiency. Model efficiency is evaluated in model calibration, which is discussed in section 2.4. Finally, model validation on Hydrochemical Facies Analyses and the fresh-saline interface is proposed in section 2.5 as methods to contribute to conventional model validation techniques.

## Metamodeling

In hydrology, a model is a simplified representation of a complex system (Clarke, 1973). A heavy computational load is often caused by expensive analysis and simulation processes to reach a comparable level of accuracy as physical testing data. To address such a challenge, metamodeling is often used (Gary Wang and Shan, 2006). Keeping these metamodels simple facilitates the involvement of stakeholders in the modeling process, the communication of associated uncertainty, and improves the credibility of its results, as recognized by (Basco Carrera et.al., 2018). Moreover, a very significant result need not correspond to an operationally large discrepancy. This can be an argument for retaining models as working hypotheses (even though the data to not agree with them), so as long as a more acceptable model cannot be found (Clarke, 1973).

A metamodel is created from the state-of-the-art groundwater flow model (henceforth referred to as “original model”) for the dune fresh groundwater reservoir near The Hague. The original model’s input and output will be used as a starting point for the metamodel. To fulfil the objectives of this study, the metamodel serves three purposes. Most importantly, the metamodel is designed to increase efficiency whilst retaining sufficient accuracy. Additionally, the model serves as a method to assess conventional modeling techniques to contribute to global efforts in coastal groundwater management.

An iterative approach is required to ensure the efficiency of a metamodel, whilst still retaining sufficient accuracy for the purpose of the original model: fresh groundwater resource management. Model calibration is done based on the original model’s input and output. Here the discrepancy between the results of the metamodel and the original model can be quantified and analyzed geo-statistically. Based on an analysis of the discrepancies between the metamodel and the original model, the metamodel can be justified to be sufficiently calibrated, to represent the state-of-the-art original model, using a similar approach in calibration. Through this iterative process, several hypotheses on model efficiency and accuracy are tested. After the metamodel can be argued to be sufficiently accurate, new methods for model validation are presented, to add to a discussion on effective modeling approaches in geohydrology globally.

## Model calibration

As stated in (Section 2.1.), the metamodel is calibrated to the original model. The method applied here is an iterative process, a feedback loop between data for calibration (output and input of the original model) and the metamodel (See Figure 4). Referring to the conceptual modeling approach (Section 2.1), this process focuses on accuracy of the metamodel, i.e., decreasing the discrepancy between the model outputs. The input and output data of both models are compared, the discrepancy is analyzed, subsequently changes are made to improve accuracy, and then the model is run again, this process is schematized in Figure 12.

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Figure 12: Model calibration. MM = Metamodel, OM = Original model

The discrepancies of the metamodel are analyzed by a comparison between the water balances, the groundwater salinity (concentration of Cl-, see Section 2.5.2), and the hydraulic heads. These model outputs are compared in a series of cross sections perpendicular to the coastline, along with an analysis of discrepancy between the two models, expressed as errors and presented statistically and spatially. These cross sections serve to investigate the function of the metamodel to represent the output of the original model on a global scale. Comparing hydraulic head distributions gives insight in flow of groundwater through the entire domain, which must also be represented by the metamodel. The extent of the cross sections is shown in Figure 13

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Figure 13: Extent of cross sections over the study area

On a smaller scale, metamodel calibration is done by comparing water balances for the study area. After regridding to a different horizontal cell size, the conductance of the infiltration ponds (see Section 2.2) is calibrated to match the water balances of the study area. Calibration on water balance is done by running steady state simulations in the metamodel and comparing to steady state outputs of the original state-of-the-art model. Another method used to compare modeled groundwater flow in the study area is the use of Flow Lower Face budgets (see Figure 13). In MODFLOW, these define the vertical flow in or out of a cell through its lower face, where the convention is that upward flow into the cell is positive, and downward flow out of the cell is negative.

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Figure 14: Flow Lower Face of a cell, side view.

For model calibration, the simulation time (39 years), starting concentration groundwater salinity and starting hydraulic heads are matched with the original model (after regridding, see section 2.3), to analyze the discrepancies between two “parallel” simulations.

## Model validation

After the metamodel has been motivated to be sufficiently efficient and accurate, new data can be introduced to assess conventional model validation techniques. In this study, the distinction between model calibration and model validation is made, to serve the purpose of the metamodel. Model calibration of the metamodel with the original model is required to minimize the discrepancy. Model validation is then used in this study to investigate further techniques to increase certainty on geohydrological model predictions in an efficient manner, minimizing effort. As predicted by (Langevin and Panday, 2012): Effective model use in the future will not only be to seek solutions but also to analyze data significance and guide further collection efforts towards minimizing uncertainty in predictions. In this chapter, the use of the fresh-saline interface and Hydrochemical Facies Analyses like (Stuyfzand, 1993) as data for model optimization will be introduced, in an attempt to contribute to the discussion on model optimization.

### Fresh-saline interface

In this study, the conceptual fresh saline interface introduced by (Oude Essink, 2001) serves as a tool to investigate the rate of artificial infiltration, acknowledging that there is a transition zone (or “brackish water zone”) between the fresh groundwater and the heavier saline groundwater due to transversal dispersion and multi-year precipitation fluctuations (Stuyfzand, 1993). For model validation, however, this concept can be integrated to gain insight in the volume of fresh groundwater, which is beneficial compared to regarding groundwater as a whole, for the objective of this study.

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Figure 16: Model validation on a fresh-saline interface (L) and on groundwater as a whole (R)

As discussed in section 1.1, the state-of-the-art fresh-saline groundwater model (the original model, OM) used by Dunea for assessing the feasibility of brackish groundwater as a groundwater resource, has only been validated on hydraulic head data. It is not calibrated on groundwater salinity and therefore neglecting validation on variable density flow, even though the model does incorporate variable density flow in the model’s groundwater flow. For the sake of argumentation, validation solely on hydraulic head data can be conceptually represented in Figure 14 (R), where there is only information on the phreatic groundwater surface level. Calibration of a fresh-saline groundwater flow model only on hydraulic head data may be right for the wrong reasons, as it doesn’t address fresh-saline groundwater regions like the conceptual fresh-saline interface shown in Figure 14 (L).

Groundwater salinity is represented in the model with chloride, as it is the dominant anion in Dutch coastal groundwater and density is linearly related to it within naturally occurring concentrations (Delsman 2015). In this study, groundwater is subdivided in terms of salinity, corresponding to (Stuyfzand, 1993):

for

for

for

Worth bearing in mind is the fact that the fresh-saline interface remains unused for the calibration of the original model. Assessment of conventional modeling techniques can, however, be done by comparing the output of the metamodel when it is calibrated to the original model, after which the MM (and implicitly the OM) can be tested to the f/s interface using the HyFA. The discrepancies between the OM and MM f/s interface output may give insight in the effects of regridding, and the added value of a HyFA for model validation.

### HyFA

The original state-of-the-art model for the fresh-saline groundwater distribution of Meijendel-Berkheijde has not been calibrated on groundwater salinity, although it incorporates variable density flow. As mentioned in section 1.2, the HyFA provides insight in the “path” that groundwater particles travel through the soil. In his study, (Stuyfzand, 1993) analyzed over 2000 samples obtained from boreholes along the coastline of the Netherlands. By sampling different depths per borehole, he could visualize the origin of various groundwater regions by their chemical composition.

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Figure 15: Cross section along coastline showing groundwater zones. Interpreted HyFA by (Stuyfzand, 1993) See Appendix A

As shown in Figure X, the geohydrology of the study domain is now not only subdivided by fresh, brackish, and saline groundwater, but also by origin. For clarity’s sake, the cross section by (Stuyfzand, 1993) was interpreted using different colors and showing relevant features only, see Appendix A for the original and interpreted cross sections. The HyFA is used for model validation by implementing origin tracers as species in MODFLOW SEAWAT. The species that are defined to validate the model output to (Stuyfzand 1993) are given in Table 1. The model simulation time is set to 40 years, which is by approximation the relative time between commencing artificial infiltration (1950) to the time when (Stuyfzand, 1993) commenced data acquisition (1990).

Table 1: Species defined for model validation, inspired by Stuyfzand, 1993)

|  |  |
| --- | --- |
| *A* | Artificial infiltration  *fresh, infiltration ponds and injected freshwater* |
| *F* | Fresh groundwater  *precipitation and infiltration through surface waters* |
| *B* | Brackish groundwater |
| *S* | Saline groundwater |

In addition to the origin and path of groundwater, the representations by (Stuyfzand, 1993) also provide information on the rate at which artificial infiltration can be achieved. For model validation, this means it can be used when examining the rate at which the depth of the conceptual fresh-saline interface increases.

## Model structure

In this section, the structure of the metamodel and the original model in MODFLOW and iMOD SEAWAT are discussed, to provide the reader with background knowledge on model features whose influence on efficiency and accuracy are studied. To avoid getting into too much detail, the scripting structure is briefly discussed in this section, further details are given in Appendix D.

### Domain and discretization

Along the coastline, the model domain ranges from Loosduinen (south), to Katwijk (north). Inlands it reaches until Zoetermeer (west). This domain discretization and the according parametrization of the original model are based on the preceding Bridging Model (Arcadis, Deltares, KWR, 2019). The original model has a horizontal cell size of 25m (Bootsma et. al. 2021). Vertically, the model top reaches the highest hydraulic heads found in the dunes (15m NAP) and reaches a depth of 250m below NAP. The top 30m of the model domain consist of 15 cells that are each 2m thick, followed by 22 cells of 5m thick and 12 cells of 10m thick. (Bootsma et. al., 2021) The vertical discretization is unchanged in the metamodel and its influence on model performance is outside of the scope of this study.

The phreatic groundwater variability throughout the model domain is schematized in Figure 5 below. For the sake of simplicity, the subsurface is represented by two aquifers and two aquitards and the fresh-saline groundwater distribution is disregarded.

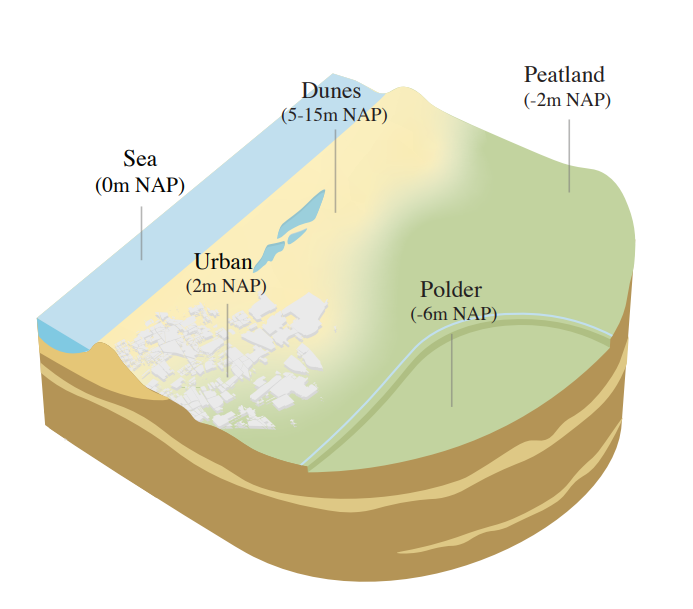


Figure 6: Model domain and piezometric groundwater head. In the dunes, the infiltration ponds can be seen.

To model the geohydrology of the domain show above, SEAWAT is used. SEAWAT is MODFLOW based and simulates 3D variable-density groundwater flow coupled with multi-species solute transport (Langevin and Guo, 2006). It is used to create cells that interact in a 3D grid. Both horizontally and vertically, this cell size can vary. These cells interact as water flows from one cell to another, based on groundwater flow equations, boundary conditions and cell parameters (horizontal and vertical permeabilities, heads, salinity) per timestep. They represent a pore volume in a soil, saturated or unsaturated with water.

+ ADD Figure of model domain and study area (since the study area is often referred to throughout the report).

### Data and coding structure

Processing of the input and output data and structuring the scripts to run the model is done in Python. Scripts and data are externally stored and managed on Github (<https://github.com/justkrantz/msc-thesis>), where the project is organized as follows (see Appendix C for the detailed script structure):

├── README.md

├── bin <- Compiled model code can be stored here (not tracked by git)

├── data

│ ├── 1-external <- Data external to the project.

│ ├── 2-interim <- Intermediate data that has been altered.

│ ├── 3-input <- The processed data sets, ready for modeling.

│ ├── 4-output <- Data dump from the model.

│ └── 5-visualize <- Post-processed data, ready for visualization.

├── reports <- For a manuscript source, e.g., LaTeX, Markdown, etc., or any project reports

│   └── figures <- Figures for the manuscript or reports

└── src <- Source code for the project

├── 0-setup <- Installing necessary software, dependencies, pull other git projects, etc.

├── 1-prepare <- Scripts and programs to process data, from 1-external to 2-interim.

├── 2-build <- Scripts to create model specific input from 2-interim to 3-input.

├── 3-model <- Scripts to run model and convert or compress model results, from 3-input to 4-output.

├── 4-analyze <- Scripts to post-process model results, from 4-output to 5-visualization.

└── 5-visualize <- Scripts for visualization of results, from 5-visualization to ./report/figures.

It should be noted that the execution of the model (resulting from initialization in Python using the structure shown above) is done through the iMOD WQ SEAWAT executable. The executables are run on an Intel(R) Core(TM) i5-5300U CPU at 2.30 GHz, with an RAM of 8,00 GB. When calculation times are mentioned in the results section, it should be noted that these are dependent not only on modeling structure but also on computer performance. However, when analyzing relative changes in calculation times for model efficiency, the effect of fluctuations in computer performance is assumed to be negligible, compared to the influence by changes in modeling structure, which will be discussed in the section 2.4.3.

### Boundary conditions

In this section, boundary conditions and their influence on the model’s efficiency and accuracy are discussed. Boundary conditions, in hydrological modeling are used either to represent a hydrological feature, or as a computational tool (Chen, 1973). In the former case, they incorporated in MODFLOW as packages (Langevin et al., 2017). Boundary conditions can be applied to a specific place (cell) and time in the model domain to represent features like lakes, infiltration ponds, or the sea. In the latter case, they can be used to make assumptions on the domain edges (see Section 2.2.3.1.) to increase the numerical model’s efficiency, while still yielding a good numerical solution if done correctly (Chen, 1973). Following this logic, when making assumptions or approaching (i.e., applying boundary conditions), one is simplifying a complex system into something less complex, and should beware of a decrease in accuracy of the model’s resulting solution. The method applied in this study regarding boundary conditions is an analysis of their effect on efficiency and accuracy in an iterative manner.

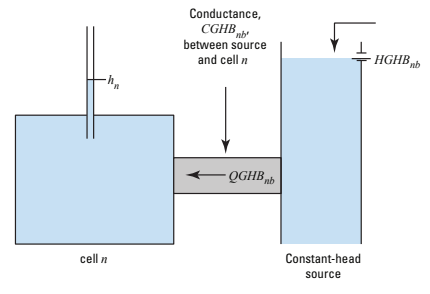


Figure 7: Diagram showing the flow between a General Head Boundary condition and its adjacent groundwater cell (Harbaugh, 2005), (Langevin et. al., 2017).

The flow between a boundary condition cell and an adjacent cell *n* representing the groundwater system, is governed by a conductance term between the two, as shown in Figure 7 in one dimension. The higher the conductance, the higher the flow between the boundary condition and the adjacent cell.

The use of boundary conditions involves empirical calibration as their use implies a simplified representation of the hydrological feature in the model. The conductance term is used to calibrate groundwater flow around the hydrological feature that the boundary condition represents. It should be recognized that use of a single conductance term to account for the resulting three-dimensional flow process is inherently an empirical exercise, and that adjustment during calibration is almost always required (Langevin et al., 2017).

* + - 1. Domain boundaries

When boundary conditions are applied to make assumptions on the model’s domain edges, their influence on the resulting solution which the model provides is analyzed. When done correctly, a boundary condition approximation can provide a good solution, as stated by (Chen, 1973). Expanding this logic to the edges of the domain on which these conditions are applied, their effect on the solution in the area of interest should be negligible in order to say that the domain edges are placed sufficiently far away. Additionally, the effect of these boundary conditions on model efficiency is also of importance for the purpose of this study. Therefore, two scenarios are run to investigate the influence of the conditions applied to the domain boundaries on model efficiency and accuracy: A fixed head (GHB), and an impermeable (no flow) boundary.

* + - 1. General Head Boundary vs River package

As discussed in section 1.2, artificially enhanced infiltration in the study area commenced in the 1950s, by engineering infiltration ponds and pumping supplementary Rhine and Meuse water into the dunes. As mentioned in Section 2.2.3., a boundary condition can be applied for cells representing infiltration ponds, rivers, and canal-and-polder areas. In this study, the difference between a fixed head boundary condition (GHB) and a variable head and drainage condition (RIV) in their effect on model efficiency and accuracy is investigated. This is done for the infiltration ponds in the study area, as for the polder area towards the west end of the domain (see Figure 6).

When implementing a General Head Boundary, a linear relation between the head of the adjacent cell and that of the GHB is established. The following relation is then solved in the system of differential equations:

Where is the flow into cell from the boundary expressed as a fluid volume per unit time (L3 T-1), is the boundary conductance (L2 T-1) and is the head assigned to the boundary condition (Langevin et. al., 2017). The flow between a GHB cell and its adjacent cell is visualized in Figure 7. In this case, intercellular groundwater flow is linearly dependent on the head of the cell, the head of the boundary condition cell and the conductance term between the two cells.

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Figure 8: QGHB flow for a general-head boundary as a function of head, h, in cell n, where HGHB is the source head and C is the conductance term for the GHB (Harbaugh, 2005), (Langevin et. al., 2017).

For a RIV boundary condition, the flow between a RIV cell and its adjacent cell is visualized in Figure 8. In this case the groundwater flow is either constant or follows a linear relation between the head of the adjacent cell and the river head. The following relation is established:

,

,

Where is the flow between the river and the groundwater system, positive if flowing out of the river (L3 T-1), is the water level (stage) in the river (L); is the hydraulic conductance of the river-aquifer interconnection (L2 T-1); and is the head at the node in the cell underlying the river reach (L) (Langevin et. al., 2017).

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Figure 9: QRIV as a function of head, h, in the cell, where RBOT is the elevation of the bottom of the riverbed and HRIV is the head in the river (Harbaugh, 2005), (Langevin et. al., 2017).

When applying a GHB condition instead of a RIV condition, a linear relation of groundwater flow on and can be used to solve a differential groundwater flow equation for a specific timestep. On the other hand, when a RIV condition is used, the flow from the boundary condition into the groundwater system is either linear, or constant, depending on , and . Therefore, the hypothesis is that the use of a GHB boundary condition for the infiltration ponds and polder areas instead of a RIV boundary condition will increase efficiency as the differential equations require less calculation time to be solved. The effect of these boundary conditions for the hydrological features mentioned on model accuracy specifically will be limitedly investigated.

* + - 1. Drainage

The drainage package in MODFLOW is designed to simulate the effect of hydrological features that remove water from the groundwater system. (Langevin et. al., 2017). This package is used to simulate surface runoff and piezometric pipe drainage in the groundwater reservoir in Meijendel-Berkheide. This boundary condition’s dependency on adjacent cell head is shown Figure 10.

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Figure 10: QDRN as a function of head in the adjacent cell. Negative QD denotes flow into the drain, out of the groundwater system (Harbaugh, 2005), (Langevin et. al., 2017).

### Input data

The model inputs for the original model (and consequently the metamodel) relevant to this study are discussed in this section. Horizontal and vertical hydraulic conductivity are parametrized with three data sources: REGIS for the deep subsurface, GeoTOP for the shallow subsurface outside the study area. The parametrization used for the TRIWACO model is also applied to the study area (Meijendel-Berkheijde), due to a higher borehole density in this specific area. GeoTOP and REGIS have a higher resolution horizontally than vertically (25 vs 100m). (Bootsma et. al., 2021)

The starting salinity of groundwater used for this model is the regridded (Section 2.3 for regridding) output salinity of a 100y simulation of the original model, which in turn used a starting groundwater salinity provided by TNO. This starting salinity is assumed to be steady state under the constant fluxes in the original model. For the starting heads, a series of steady state calibration steps were performed (Section 2.4). For the precipitation influx, the mean of the daily precipitation used for the original model is used. The pumping rate from the reservoir, for drinking water is represented in the Well and DRN packages, in accordance with the original model. For model calibration and validation, the inputs will be discussed in the respective Sections 2.4 and 2.5.

## Regridding

Increasing efficiency of a model by decreasing calculation time is one of the main subjects of this study. Decreasing the number of equations to be solved in the system of equations may be an effective approach. By increasing cell sizes but maintaining the same model domain, the number of cells, and consequently the number of equations in the system of differential decreases, thereby reducing the calculation times (leaving all other features unchanged).

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Figure 11: Diagram showing regridding process: upscaling cell dimensions & hydraulic conductivities

As shown in Figure 10, regridding to a larger cell size changes the cell volume. When regridding, hydraulic conductivities, governing intercell groundwater flow, should also be accounted for. In the case of Figure 10, replacing 9 cell parameters with one cell parameter reduces 9 groundwater flow differential equations to be replaced by one.

Where represents individual cell flows in the initial cell discretization (L3 T-1) and represents flow through the replacing regridded cell (L3 T-1). To increase efficiency, whilst retaining accuracy, the regridded flow should be equal to the initial flow when the hydraulic head gradient is constant. The relation that should be satisfied becomes:

Rearranging gives:

In the case described above, the regridded hydraulic conductivity should be the sum of all hydraulic conductivities it replaces, to represent the same flow of groundwater. A geometric mean is the most robust method to rescale hydraulic conductivities (Bootsma et. al., 2021). As the number of cells decrease, the model becomes a more simplified representation of a physical process, which may come along with the risk of losing accuracy. The effect of horizontal cell size on model calculation times is investigated (by changing from a cell size of 25m for the OM to 250m for the MM) but changing the vertical cell size and using variable horizontal cell size throughout the domain are outside the scope of this study.

# Results

The results described in this section show the effects of applying conventional modeling techniques on model efficiency and accuracy, as described in Section 2. The method applied is partially iterative (Section 2.2), intermediate calibration results are omitted in this chapter (to be found in Appendix D), intending to present the results as concise as possible. First, the effect of the applied methods on model efficiency is described in Section 3.1. Subsequently, the methods’ effect on accuracy is described in Section 3.2 to form the basis for an analysis on the discrepancies between the metamodel, and original model. These discrepancies are described in as indicated by the water balance, hydraulic heads, and groundwater salinity. Section 3.3 show the model results against the Hydrochemical Facies Analysis. Further interpretations of these results, and discussions can be found in Chapter 4.

## Model efficiency

By changing the cell size from 25x25m to 250x250m horizontally, and leaving the vertical cell size unchanged, the elapsed run time for a 100y simulation is 2h53min with a no flow boundary condition at the edges of the model domain, and 14h5min for a fixed head boundary condition respectively.

By applying a GHB condition to the infiltration ponds as and polder area and changing the horizontal cell size to 250x250m, the calculation time required to solve the system of differential equations decreased to 1:33 hours.

The effect of choosing between a GHB and RIV boundary condition for the infiltration ponds and polder areas on model efficiency has not been investigated explicitly. However, the simulation time of the resulting metamodel has drastically been decreased for a 39 year simulation, with respect to the original model.

The hydraulic head errors in the study area remain unchanged, therefore the model domain edges are assumed to be placed sufficiently far away to have negligible effect on the accuracy of the model.

+ mention effects of changing BC’s

## Model accuracy

In this section, the discrepancies between the original model and metamodel output is presented and described

### Hydraulic head distribution

The hydraulic head distribution of a parallel metamodel and original model simulation of 39 years can be seen in Figure 14. In CS1, CS2, CS3, the regional groundwater flow from the sea and dunes (high hydraulic heads) on the left, to the polder areas (low hydraulic head) is represented in both the original model and metamodel output. Additionally, the range of hydraulic heads visible in the model domain are of the same magnitude

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Figure 17: Cross sections perpendicular to coastline, after 39 years. OM = Original Model, MM = Meta Model

To investigate the discrepancy statistically, the output of the OM was regridded to the same cell size of the MM, after which an error could be calculated. The global mean error on hydraulic heads through the entire domain is calculated to be , with a standard deviation of .

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Figure 18: histogram showing hydraulic head error of the MM, compared to the OM

For the study area, the mean error on hydraulic heads is , and . The histogram of the error between the MM and the OM the study is shown in Figure 19. As can be seen in the histogram, most cells of the MM have a lower hydraulic head than the cells at the same location in the OM. The highest largest number of cells of the MM have a hydraulic head that is around 0.25m lower than the OM. The positive peak in the histogram shows that the MM has a fraction of cells which hydraulic heads are about 0.5m higher than the heads of the same location in the OM.

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Figure 19: Histogram of steady state hydraulic head error in the study area

In Figure 20, the variability of the error of the metamodel with the original model for steady-state heads is shown for the top 30m (Figure 20b) and for the entire depth (Figure 20a). It shows that the largest errors in the study area are found in the top 30m. Here, the steady-state hydraulic heads calculated by the metamodel are lower than those calculated by the original model.

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Figure 20: Top view plot showing mean absolute errors over depth for the steady state hydraulic heads, of the metamodel with the original model. Mean absolute error over entire depth (top, a), and mean absolute error over top 32.5m (bottom, b). The study area lies along the coastline between Scheveningen and Katwijk.

### Groundwater salinity

The groundwater salinity of the OM and MM are shown in parallel cross sections, perpendicular to the coastline (see Figure 13) in Figure X. As discussed in Section 2.2.4, the groundwater salinity is represented by the concentration of Chloride (see Section 2.2.3. Input and output). In it, the effects of variable density flow can be seen. Generally, the fresh groundwater lies on top of the heavier saline groundwater.

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Figure 21: groundwater salinity of metamodel (MM) and original model (MM)

### Water balance

After the global calibration is deemed sufficient, the cell budgets and intercell flows are used to calibrate the conductivity below the infiltration ponds (represented as General Head Boundary condition, see Section 2.2.2.2.) to the water balance in the study area. Figure 17 shows the water balance of the study area in the OM to which the conductance of the infiltration ponds is calibration (see section 2.2.1 for study area). After six iterations, the conductance term below all GHB cells inside the study area in the MM have been decreased to a factor of 0.625 to match the water balances.

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Figure 22: water balance of the study area in the original model (OM)

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Figure 23: Steady state water balance for the study area for the metamodel (MM) after 6 iterations on conductance (cond6)

Vertical flow through the lower face of a cell can be summoned from the model output through flow lower face budget values. As described in section 2.4., the convention describes that upward flow through the lower face of a cell is positive, and accordingly downward flow through the lower face of a cell is negative. Figures 22 and 23 show the error that the metamodel has for flow lower face budget values, compared to the original model. For an elaboration of the term “Study area”, see section 2.2.1. Globally, the mean vertical flow downward is lower in the metamodel than in the original model. In the study area, the mean vertical flow downward is higher in the metamodel than in the original model. The standard deviation is higher in the study area than in the global model domain.

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Figure 24: Flow lower face error global

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Figure 25: Flow lower face error for study area

## Model validation on groundwater salinity

### HyFA: Cross section along coastline

Figures 22 and 23 show how the origin tracers in the metamodel compare to the HyFA. The depths to which the artificially enhanced infiltration reaches is about 80m. The brackish water zone is about 20m depth in both. The shape of the artificially infiltrated groundwater by the metamodel differs from that of (Stuyfzand, 1993), as there is a region of “native” fresh water in between two “alien” infiltrated water bodies. The horizontal extent corresponds globally, although the overall shape varies between the two.

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Figure 26: Cross section with origin tracers along coastline, interpreted version of cross section by (Stuyfzand, 1993)

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Figure 27: Metamodel output showing species after a 39y simulation

### HyFA: Cross section perpendicular to coastline

Figures 24 and 25 show the groundwater origins on cross sections perpendicular to the coastline. The depth to which artificial infiltration reaches in 40 years is slightly lower in the metamodel output (-60m) , compared to the HyFA (-80m). The horizontal extent and global shape of the artificially infiltrated groundwater are represented by the metamodel. The shape of the fresh-brackish and the brackish-saline interfaces in the metamodel coincide globally with those in the HyFA.

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Figure 28: Cross section perpendicular to coastline (Stuyfzand, 1993)

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Figure 29: Cross section perpendicular to coastline

### Fresh-saline interface

In Figure 26, the depth of the fresh-saline interface is shown (see section 2.5.2). The metamodel fresh-saline interface has a comparable overall shape, relatively deep near Scheveningen and shallower further inland at the edges of the model domain. Along the shoreline, the metamodel has a deeper fresh-saline interface than the original model. The largest errors can be seen near Voorschoten (60m higher in the metamodel than in the original model output) and near the southern edge of the domain, which South of The Hague. It should be noted that the study area lies between Scheveningen and Katwijk.

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Figure 30: Fresh saline interface after parallel 40y simulations, original model (top, a), metamodel (middle, b), and the absolute error of the metamodel with the original model (bottom, c). The Study area is located between Scheveningen (South) and Katwijk (North)

For the study area (see section 2.2.4.), the original model and metamodel’s fresh-saline interface development over time can be seen in Figure 27. The original model fresh-saline interface becomes less shallow in 40 years and moves to an equilibrium at around -63m, whereas the metamodel shows an increase in depth and continues to increase more in depth at -70m after 40 years, when subjected to the same fluxes.

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Figure 31: Development of fresh-saline interface in the study area over two parallel 40y simulations, original model and metamodel.

# Discussion

Are the results sufficient to answer the research question? Is the objective of the study fulfilled?

## Model efficiency

A critical review of the results obtained from this study includes acknowledging the fact that the effect of applying a GHB vs RIV boundary condition for the infiltration ponds and polder areas on model efficiency has not been investigated explicitly. However, the simulation time of the resulting metamodel has drastically been decreased for a 39y simulation, with respect to the original model (40 days for a 1000y simulation). The accumulated effect of methods applied may be considered as effectively increasing model calculation efficiency.

## Model accuracy

### Domain edges

Model domain edges

The hydraulic head errors in the study area remain unchanged, therefore the model domain edges are assumed to be placed sufficiently far away to have negligible effect on the accuracy of the model.

### Variable groundwater flow in the study area

### Flow lower face (FLF)

The metamodel seems to have higher vertical flows downward in the study area than the original, as indicated by the lower FLF budget values (Section 3.2.3) and the fresh-saline interface increasing in depth. These budget values for vertical flow are calculated as a mean over depth and the study area. Figure 32 shows the horizontal mean absolute error over the study area (horizontally) vs depth. Until a depth of -77.5m, the metamodel calculates a higher vertical flow downwards than the original model (by convention, see section 3.2.3), for depths greater than -77.5m, the metamodel calculates a relatively lower flow downwards than the original model.

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Figure 33: FLF mean absolute error over study area vs depth

The original model has been constructed using a fixed head boundary at the edges of the domain. Results have shown that this is of no influence on the model accuracy inside the study domain. The original model has higher calculated steady state heads in the study area, than the metamodel, calculated as a mean over depth, as shown section 3.2.1. However, the average error of hydraulic heads over the study area vs depth shown in Figure 34, shows that the hydraulic heads are in accordance with the FLF budgets (Figure 33).

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Figure 34: Steady-state hydraulic heads error over study area vs depth

### Fresh-saline interface and groundwater salinity

The higher downward flow of the metamodel is consistent with the rate at which the f/s interface increases in depth with respect to the OM as shown in Figure 31. A possible reason could be the boundary conditions applied at the edges of the domain. In the OM, the edges of the domain are set as a constant head boundary. This could lead to an underestimation of the depth of the f/s interface (WHY?). On the other hand, an impermeable boundary at the edges of the domain could lead to an overestimation of the f/s interface. However, changing the boundary conditions at the edges of the domain showed no difference in f/s interface development, proving the hypothesis that they are placed sufficiently far away from the study area.

Moreover, the original model has not been calibrated on groundwater salinity (see Section 3.2.), and although the MM (which has been calibrated to the OM in water balance, hydraulic head distribution) does show semblance with the HyFA, (see Section 3.1), this does not necessarily mean that the OM’s f/s interface is in fact, closest to the actual f/s interface, despite its smaller cell size and consistency with the FLF and head data.

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Figure 35: 100y MM simulation showing origins of groundwater, CS along coastline

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Figure 36: 100y MM simulation showing origins of groundwater, CS perpendicular to coastline

Figures 35 and 36 shows the groundwater origin distribution after a 100y simulation. Along the coastline, the depth of artificial infiltration remains the same as after a 40y simulation (Figure 27). On the cross-section perpendicular to the coastline (Figure 36), the shape of the artificially infiltrated groundwater region has changed with respect to the 40y simulation (Figure 29). Horizontally, it spreads out 1km further inlands, following the regional hydraulic head gradient (Figure 17). Vertically, the artificially infiltrated water reaches more than 10m deeper after 100y. The f/s interface also appears steady over time in the presented cross sections in Figures 35 and 36.

In this study, the fresh-saline interface is calculated as the minimum depth at which the groundwater salinity becomes brackish (see Section 2.5.2). However, as seen from the CS3 and CS4 from the groundwater salinity cross sections perpendicular to the coastline presented in Figure 21, in the OM, the saline groundwater intrusion occurs at a shallow depth, below which there is more fresh groundwater. Therefore, calculating the fresh-saline interface here as the minimum depth at which groundwater becomes brackish or saline, leads to an underestimation of the actual fresh-saline interface depth that lies below this intrusion zone. This intrusion may disrupt the fresh-saline interface development in the OM shown in Figure 31, as the actual fresh-saline interface below the shallow intrusion still increases in depth. A shallow intrusion zone near the coastline also recognizable in the cross section of (Stuyfzand, 1993) in Figure 27, with similar extent (100s of m) but is unrepresented in the calculated metamodel groundwater salinity.

An analysis of variable density flow may provide further insight in the discrepancy between the original model’s shallow intrusion and its absence in the metamodel. The general form of Darcy’s law for variable density conditions may be rewritten as (Bear, 1979; Senger and Fogg, 1990; Langevin and Guo, 2006):

Where [LT-1], **k** is the permeability tensor [L2], is the dynamic viscosity [ML-1T-1], is the freshwater head [L], is pressure [ML-1T-2], is the gravitational acceleration [LT-2], and is the upward coordinate direction aligned with gravity. This relation shows that horizontal flow components can be directly evaluated from the freshwater head, and vertical flow components can be calculated from the second term inside the parentheses (buoyancy term, Holtzbecher 1998, Oude Essink, 1998). The vertical buoyancy term can be of similar magnitude as the horizontal component, and the effects of relative viscosity are neglected in SEAWAT (Langevin and Guo, 2006).

To get the horizontal component of variable density in accordance with Equation X, the intrusion shown in OM results need not be incorrect with respect to the actual groundwater intrusion that occurs, despite neglection of calibration of the OM on groundwater salinity data, since the horizontal flow component of variable density flow can directly be calculated from the hydraulic head gradient. However, the vertical component of variable density flow is dependent on groundwater density (thus groundwater salinity) in the buoyancy term. Since the OM has not been calibrated on groundwater salinity data, vertical variable density flows may not be well represented by the model.

Extending the metamodel’s simulation time to 200y gives the development of the f/s interface shown in Figure 32

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Figure 32: Development of fresh-saline interface over 200 y simulation

### Effects of regridding

In the context of this study, it could be stated that a model’s empiricism is inversely proportional to its scale, as discussed in Section 2.1. By increasing the model’s cell size, its capability to predict small scale groundwater flows decreases. The shallow groundwater intrusion that is unrepresented in the metamodel may be a large-scale effect resulting from accumulation of small-scale groundwater flows that the coarse metamodel fails to capture. Other features that the metamodel could fail to represent is the small-scale radial flows which occur around canals.

## Model empiricism: accuracy and efficiency

A model is a simplified representation of a complex system (Clarke, 1973). The metamodel produced could therefore be seen as a superlatively simplified representation of a physical system. The discussion in Section 4.1 has contributed to the value of these discrepancies and where they come from, but uncertainties remain as to where these discrepancies come from. Moreover, if these are small enough to argue that the proposed model adjustments are sufficient to retain sufficient model accuracy.

To shed another light on this question, the problem can be approached from a theoretical point of view, by discussing hydrological models’ predictive capacity for a physical process. In their study on model types for hydrology purposes, (Clarke, 1973) makes the distinction between *conceptual* models and *empirical* models, according to whether (conceptual) or not (empirical) they incorporate the physical process acting upon parameters to produce the output variables. (Clarke, 1973)’s discussion will be applied to the metamodel to contribute to developing a modeling approach that consistently approaches its predictive capacities in this section.

They argue that many models that are conceived as conceptual models are based on empirically derived parameters. Conversely, many empirical models have components that are conceptual. This distinction is made to address the feature that all models have in common: their predictions differ from the actual physical processes that occur (Clarke, 1973). Moreover, distinction between empirical end conceptual modeling features may help in checking consistencies in assumptions on which the model relies, and to account for the discrepancies a model produces, compared to observations (Clarke, 1973) or original model outputs for metamodels.

Regridding the discretization of the original model to a coarser grid size, and calibrating to the cumulative effect on water balances or hydraulic heads is an empirical practice since it loses the conceptual value of small-scale variations in groundwater flow or subsurface characterizations. This, in turn, may lead to accumulation of errors when increasing the model’s empiricism. However, the empirically determined law of Darcy (Clarke, 1973) is by Oxford Definition empirical: Based on experiments of experiences, rather than ideas or theories (Oxford University Press, n.d.).

If the logic applied above is accepted, then any mathematical groundwater model using Darcy’s law for subsurface flow is to some degree empirical. Furthermore, the development of the fresh-saline interface, which may appear to diverge the most between metamodel and original model outputs, is a geohydrological feature on which the original model has not been calibrated. It therefore remains unknown which of the two model has the highest predictive capacity for modeling the development of this geohydrological feature.

An important factor that remains to be addressed is the effort required to create a model. As effort required to set up a model requires a professional’s time, model efficiency is also linked to efficient modeling practices. A model that has a high predictive capacity, but whose approach is difficult to apply to other geohydrological problems is of less value in the context of this study, since the assessment of conventional modeling approaches to contribute to groundwater management issues globally requires applicability overall.

## Hydrochemical Facies Analyses for model optimization

As argued by (Langevin and Panday, 2012), we can improve our groundwater models with more advanced modeling programs, faster computers, and better calibration strategies, but without better quality data and more of it, improvements in our models and their predictive capabilities will be modest. A feasible investment for site specific models for groundwater management support may therefore be the acquisition of quality data. A balance between efficiency and accuracy may be easier obtained when introducing data to the model like the HyFA.

The Hydrochemical Facies Analysis shows as notable difference with the modeled groundwater distribution using origin species (Section 3.3.1.). The model results show two unconnected infiltrated groundwater regions, whereas the HyFA of (Stuyfzand, 1993) shows these artificially infiltrated groundwater regions are connected. Although unmentioned in his study, the horizontal sampling interval can be derived from Appendix A. 12 boreholes over the conservative approximation of a distance of 12km between Scheveningen and Katwijk, correspond to a conservative sampling interval of ~1km. The interpolation necessary to create a description of the subsurface as presented by (Stuyfzand, 1993) from data acquired with a sampling interval of 1km, could mean that this feature is represented well in the modeled groundwater distribution and unrepresented in the HyFA distribution.

Nevertheless, the value of the HyFA as a tool to study the “path” of groundwater has proven to be fruitful for model validation by the results of this study. By using species (Section 2.5.2.), the model was able to reproduce a volume of artificially infiltrated fresh groundwater with the same order of magnitude as the HyFA. This confirms the hypothesis that HyFA is valuable for model validation over a relatively short time span.

Coming back to the statement by (Langevin and Panday, 2012) on the future of groundwater modeling: “[In the future] we will use models more effectively to not only seek solutions but also analyze data significance and guide further collection efforts toward minimizing uncertainty in predictions”, the significance of groundwater salinity data and HyFA have proven to be insightful for investigating a coastal fresh groundwater reservoir. When the efforts of (Stuyfzand, 1993) are incorporated in an early phase of a project, and groundwater samples are acquired simultaneously with collection of hydraulic head data and groundwater salinity data from boreholes, the use of HyFA combined with a modeling practice described in this study may be feasible to incorporate in groundwater modeling practice. For the aim of the original model (investigating the feasibility of brackish groundwater as a source of drinking water), early incorporation of the HyFA data to the model may have inferred the use of an even larger horizontal cell size.

## Quasi-paleo-modeling

Proposed as a way out of the density feedback of solute concentration on groundwater flow by (Delsman, 2015), the use of paleo-modeling can be applied to mitigate the difficulties in choosing an initial concentration to start form. By placing the starting point in time sufficiently far away, its influence on the current state diminishes. Moreover, (Delsman, 2015) argues that neither the salinity distribution nor the hydraulic head distribution was, in their paleomodel, at any point in steady, state and that the assumption of steady state on present-day conditions is not warranted for coastal aquifers as the one considered in his research. The author of this study by no means wishes to question these statements and findings, rather add to the discussion on what modeling approach to apply when considering coastal aquifers like the one studied in both (Delsman, 2015) and this study, with the purpose of contributing to sustainable groundwater management efforts globally.

As mentioned in Section 1.1 in areas where extensive human intervention (like extraction of groundwater) takes place, the anthropogenic influence on fresh-saline distributions may become primary, on a much smaller timescale (Oude Essink, 2001). The metamodel results show that a similar fresh-saline interface with an artificially infiltrated volume of groundwater with an order of magnitude similar to that obtained in the HyFA could be obtained using a modeling approach which required a much smaller timescale than a paleo-timescale.

Moreover, as acknowledged by (Delsman, 2001): calibration and a rigorous sensitivity analysis could not be performed, due to the lack of data on such a long timescale and therefore calibration could only be done on the most recent periods. As for this study, it could be argued that a more rigorous calibration or sensitivity analysis could have been done, although the problem with choosing an initial groundwater salinity distribution would then still remain.

This study has shown that validation on a shorter timescale is possible, for the purpose of investigating the artificial infiltration in the dune reservoir, occurring on unnaturally short timescales, adding to the validity of the hypothesis of (Oude Essink, 2001). By using the resulting salinity of a 100y simulation of the original model as starting salinity, the method used could be regarded as quasi-paleo-modeling. This method acknowledges the fact that the coastal aquifer considered is at no point in steady state (Delsman, 2015), but makes use of a shorter simulation time to increase calibration possibilities. As for steady state boundary conditions, this discussion remains restricted. Further research may be necessary to investigate the possibilities of quasi-paleo-modeling.

# Conclusion

List the objectives, the research questions, the answers.

# Recommendations

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# Appendix A: Original hydrochemical longitudinal cross section, longitudinal along coastline

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# Appendix B: Original hydrochemical longitudinal cross section, perpendicular to coastline

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# Appendix C: Detailed script structure

# Appendix D: Intermediate calibration results