Geochemical modelling of reactive transport processes with deep neural networks

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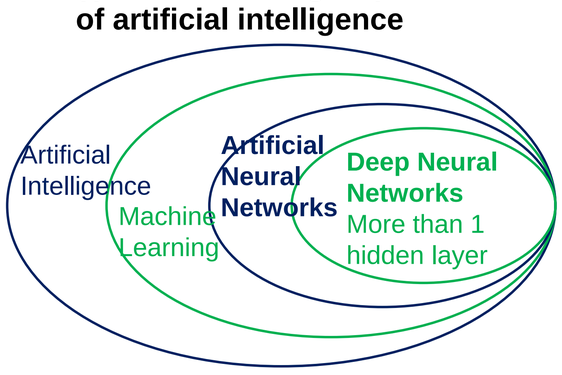
Introduction

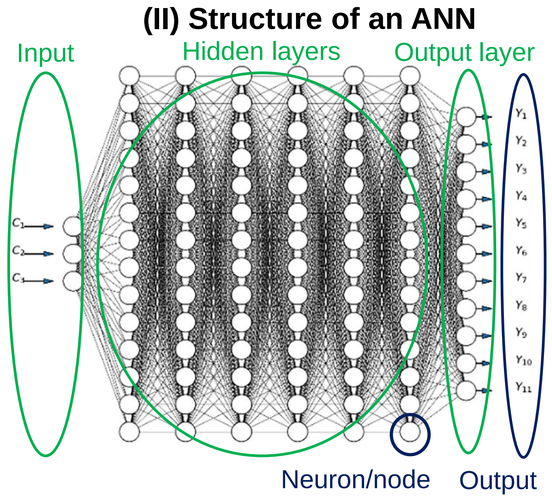
Reactive Transport Modelling is a powerful tool for the investigation of geochemical processes and phenomena. Typically, the modelled system is discretized into reaction cells (voxels), in which the chemical speciation and phase equilibrium is calculated at each simulation time step, followed by a mass transfer step between the cells. The speciation can be calculated with a geochemical solver, such as PHREEQC or GEMS. Such calculations are very time consuming in comparison with the mass transport step, and force the user to simplify the modelled system. A possible solution to speed up these calculations could be the usage of artificial neural networks, which can be trained to forecast the geochemical speciation (output) based on a certain input (e.g. amount of dissolved elements).
This master thesis aims to study the performance end efficiency of artificial neural networks (ANN) for geochemical modelling and to evaluate the quality of the resulting reactive transport modelling. Furthermore, a comparison between different ANN structures and their accuracies for geochemical calculations in systems of different complexity shall be made.

Methods

(I) ANN as a subgroup of artificial intelligence

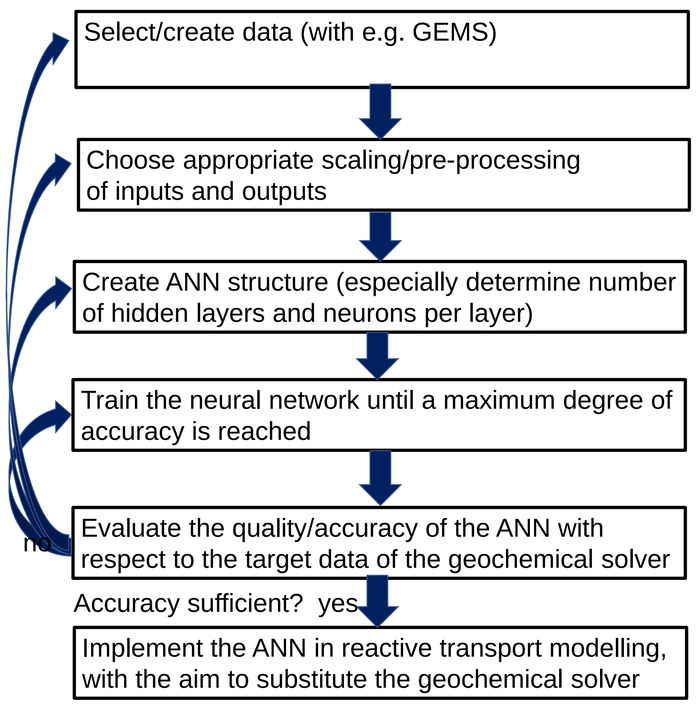


(II) Structure of an ANN



- Input/Output: Matrices of data; an ANN is trained to predict an output based on a given input
- Neuron: Smallest computational unit; consists parametrised mathematical functions, whose coefficients are optimised during training
- Layers: Set of neurons; one training epoch starts at the first hidden layer and updates the values of the neurons of all subsequent layers until the last layer (output layer) is reached

(III) From raw data to a reactive transport modelling implementation



- ANN need to be trained for each geochemical system in an iterative, time-demanding process
- Well designed and trained ANN give accurate predictions and are still small enough to provide a considerable speedup compared to the geochemical solver

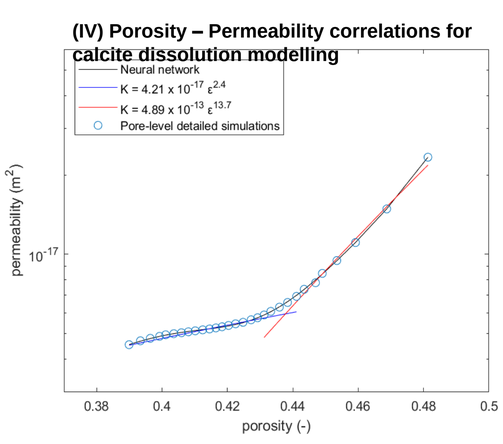
Results

Three systems of increasing complexity are presented to show potential usage of ANN for reactive transport modelling. The first two systems are described in detail in (Prasianakis, Haller, et al., 2020), while the results of the last one have not yet been published.

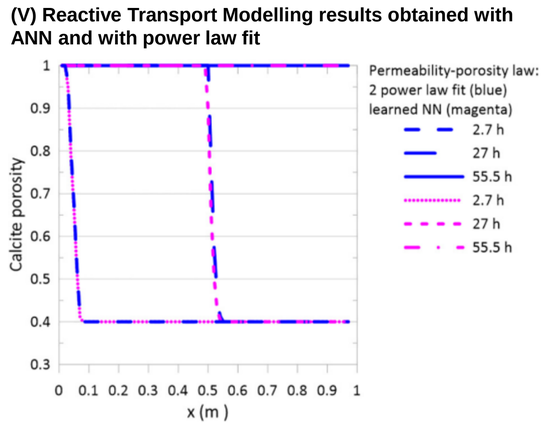
Case 1: Calcite dissolution

- **System:** Pore-scale simulations of calcite dissolution result in a permeability-porosity relationship, which can be used for upscaling in order to evaluate macroscopic parameters. The system is described in more detail in (Prasianakis *et* al., (2018).
- **ANN benefits:** No manual fitting required and easier upscaling
- **Data:** Porosity (input) and permeability (output), from microscale-simulations
- **ANN structure:** Simple, only one hidden layer with five neurons
- **Accuracy:** Excellent (see figures below)

(IV) Porosity – Permeability correlations for calcite dissolution modelling



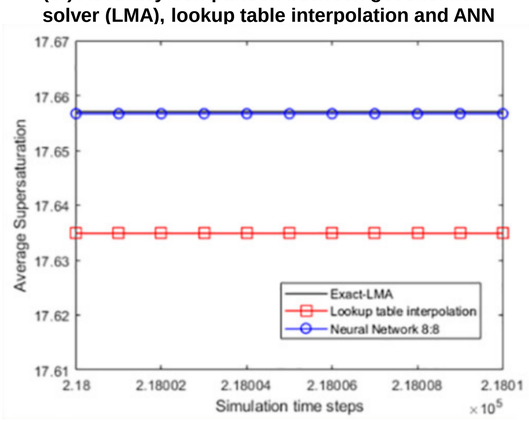
(V) Reactive Transport Modelling results obtained with ANN and with power law fit



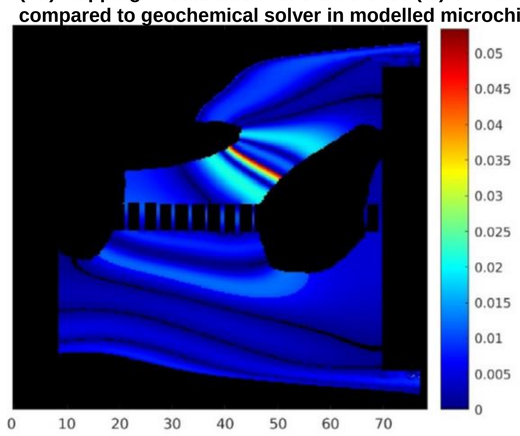
Case 2: Lab-on-a-chip experiment

- **System:** An experiment in which celestine dissolution and precipitation in microchips is controlled by the inflow of SrCl2 and Na2SO4. Reactive transport simulations help to quantify where and how much celestite precipitates/dissolves by calculating the saturation index of celestite. See (Poonoosamy et al., 2019) for more details.
- **ANN benefits:** Several orders of magnitude speedup of the modelling compared to GEMS
- **Data:** Input: dissolved Sr and S; Output: saturation index of celestite
- **ANN structure:** Slightly more complex: two hidden layer with eight neurons each
- **Accuracy:** Excellent (see figures below)

(VI) Accuracy comparison between geochemical solver (LMA), lookup table interpolation and ANN



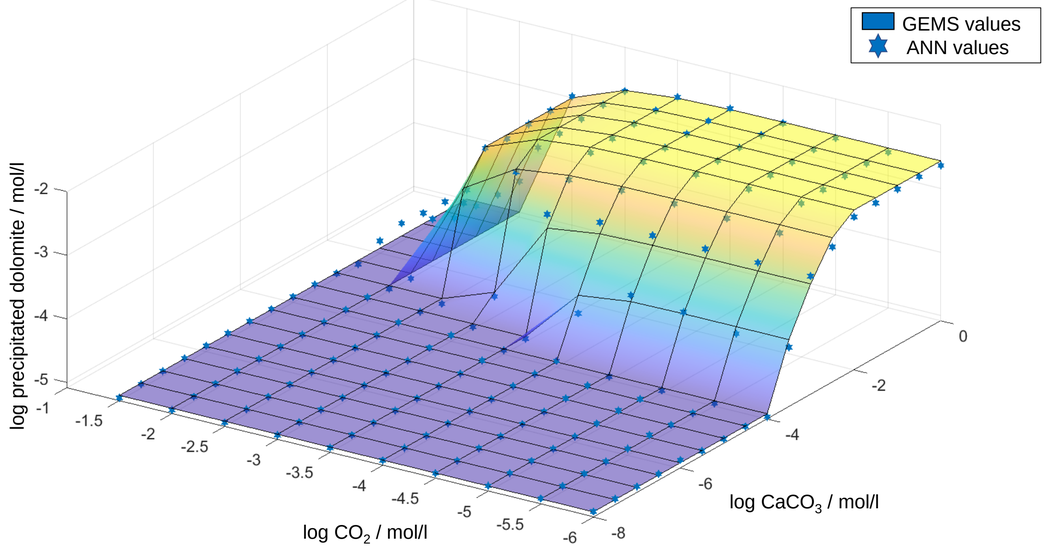
(VII) Mapping of saturation ratio difference (%) of ANN compared to geochemical solver in modelled microchip



Case 3: Calcite/dolomite precipitation and dissolution

- **System:** A more advanced system compared to case 1, including aqueous species and mineral precipitation. It can be used to evaluate e.g. the interaction of groundwater with a limestone. An application can be seen e.g. in (Guérillot & Bruyelle, 2019).
- **ANN benefits:** Considerable speedup compared to a geochemical solver
- **Data:** Input: dissolved $CaCO_3$, $MgCl_2$ and CO_2; Output: aqueous speciation of Ca, C, Mg and Cl, pH and precipitated calcite and dolomite
- **ANN structure:** Four hidden layers with 25 neurons each (see image in methods section)
- **Accuracy:** Varying, depending on output species; not sufficient for e.g. precipitation of dolomite (see figure below)

(VIII) Prediction of precipitated dolomite, with constant $MgCl_2$ concentration



Discussion & Conclusions

- Artificial neural networks can be trained to give reliable predictions for simple systems (like case 1 and 2 in the results section). Systems with multiple inputs and outputs, however, could not entirely be described by ANN so far.
- Small ANN (with only few hidden layers and neurons) provide faster calculations, while larger ANN are often able to provide better accuracy. For the quite small ANN of the lab-on-a-chip experiment, a speedup of up to 10^4 has been achieved compared to full geochemical speciation calculations with GEMS. In other words, if GEMS made 0.001M predictions/s, an ANN would make approximately 10M predictions/s. This enormous speedup is so far the biggest advantage of using ANN in reactive transport modelling.
- It might be time consuming to create and train an ANN, since a new ANN needs to be trained for every different system. However, suppose a geochemical calculation requires 1 day with a trained ANN, then the few days or weeks of training are only a small fraction of the 27 years GEMS would need instead for the calculation. The potential of ANN for more complex geochemical systems is currently still under exploration; however, a lot of progress in ANN and machine learning in general has been obtained in the last few years and even more will certainly be made in the recent future.

Acknowledgments

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- Figures IV to VII: Prasianakis, Haller, et al., 2020