Multivariate mixing calculations used to trace modern Baltic Sea water intrusion at Äspö, Sweden

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The Swedish Äspö Hard Rock Laboratory (HRL) is located under a small island off the Baltic coast approximately 350km south of Stockholm. The Äspö HRL was initiated by the Swedish Nuclear Fuel and Waste Management Company (SKB). Äspö is being investigated because it geologically represents a variety of typical granitic crystalline bedrock environments in Sweden designated as suitable host rocks for the final disposal of radioactive waste.

Many boreholes have been used to evaluate the geological, hydrogeological and hydrogeochemical character of the Äspö area. In order to establish the mixing portions in the groundwater a *Multivariate Mixing Model* was constructed (Laaksoharju et al. 1994). The model describes how large portions of a particular type of water are needed in order to explain the chemical composition of the observed water. The mixing processes are inherently very complex and include multi end-member mixing processes. A multivariate method called Principal Component Analysis (PCA) was therefore used. The strength of this approach is that all variables in a data matrix can be examined simultaneously. Greater resolution is possible and the character of the data in a general data matrix is therefore more easily identified than using univariate analysis, where only one variable is compared at a time. The major components Cl, Ca, Na, Mg, K, SO_4 HCO_3 and the isotopes ^2H, ^{18}O and ^3H were used in the Principal Component Analysis. It is important to note that both conservative and non-conservative elements were used. This is possible since conservative or non-conservative behaviour in one or several of the variables can be tracked by PCA.

The result of the analysis and the identified end-members are shown in Figure 1. The selected end-members represent extreme waters found in the Äspö area. The *Glacial* end-member has been determined as an old glacial water based on the stable isotope values which indicate cold climate recharge (^{18}O= -15.8 SMOW) (Smellie and Laaksoharju, 1992). *Deep Saline* water represents a brine type of water found at 1700m depth, *Baltic sea* water represents modern Baltic sea water. *Modified Baltic Sea* water represents Baltic sea water which has been modified by chemical process such as sulphate reduction. *Shallow* water represents relatively modern non saline groundwater.

The five identified end-members form a pentagon. The observations within the pentagon can by definition be described by the selected end-members. The co-ordinates for the observations are given by the first and second Principal Component respectively (Comp 1 and Comp 2 in Figure 1). The scales in Figure 1 are linear and the distance from any observation to the five end-members can be calculated by using simple trigonometric functions ie, the pentagon is used as a phase diagram. The distance is equivalent to the mixing ratios of any water observed in the system. The exact mixing portions of any groundwater sample can be calculated.

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Infiltration of modern Baltic Sea during the construction of the underground laboratory has been modelled (Figure 1) as an example of how the method can be applied. By using the described technique the mixing portions for all the observations at Äspö can be calculated and the feasible end-members can be identified (Laaksoharju and Skårman, 1995).

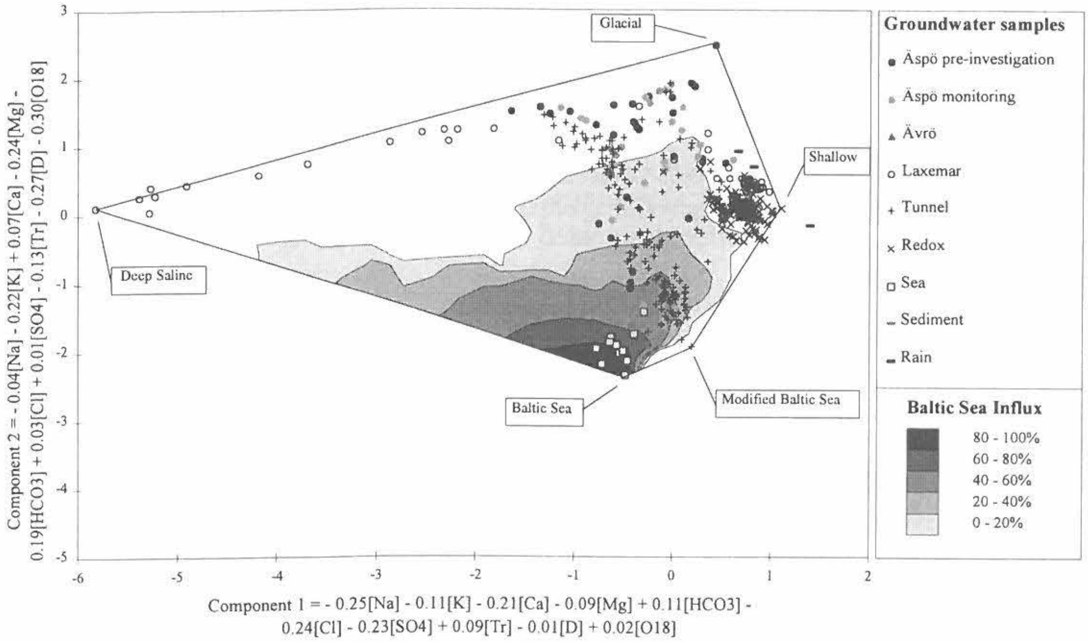

***Figure 1**: Principal Component plot used for identifying end-members in the Äspö area and to calculate the influx in portions of 100-80%, 80-60%, 60-40%, 40-20% and 20-0% of modern Baltic Sea water. The position of the selected end-members are shown in the figure. Between the five end-members lines are drawn so that a pentagon is formed. The observations within the pentagon can by definition be described by the selected end-members. The pentagon is used as a phase diagram. The mixing ratios of any observed water can be calculated.*

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