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Water Quality Mixing Analysis Using a Hilbert Space Setting

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❑ Abstract

- A Common problem occuring in the analysis of water is the relative proportions of considered constituents found in surface water or groundwater. This problem occurs when analyzing groundwater with respect to the source of pollution observed in sampling data over time.

- If one or more sources of pollution is under scrutiny, chemical "fingerprints" can sometimes be determined at the source locations, which can then be used to resolve sampling data at the point of interest into the proportions of contribution from the suspected sources.

- A method to accomplish the apportionment of source contribution, is to utilize the Hilbert space setting, where the determined chemical fingerprints are the basis vectors of a Hilbert space, with the inner product defined to be the usual vector dot product.

- To demonstrate the procedure a case study is examined involving 214 samplings and 26 wells.

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❑ Introduction

- A municipal production groundwater well was found to show increasing levels of total dissolved solids (TDS), starting at or before 1985, resulting in the groundwater well being shut down once the TDS levels became unacceptable, causing, among other effects, impacts to industrial use cooling towers.

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- Groundwater sampling data had been collected from a variety of wells for a period of nearly 20 years, and it was contemplated that these data could be used to determine the source of the TDS contamination at issue, and to determine the relative contribution of the sources if there were more than one significant source.

- Because TDS is well-known to be conservative, chemistry effects were assumed to be negligible.

- To proceed with the analysis, chemical makeup star diagrams of the TDS were developed for the 214 well samplings, which included well samplings at or near possible sources of the TDS.

- The underpinnings in the use of star diagrams are well-known (e.g., program: SEQUENCE by Rockware, Inc., www.rockware.com, or www.waterloohydrologics.com.

- From an analysis of groundwater levels of the unconfined aquifer, the flow field was determined and, from the chemical analysis, the region of elevated TDS ratings was identified.

- Because the flow field was determined to remain stationary in time, the identified region of elevated TDS measurements became the focus of the study.
- The boundary of the region of interest was determined to be consistent with the TDS measurements, in that measurements of the groundwater from wells located outside of the region boundary were found to have TDS readings that were essentially identical, and *remained nearly unchanged over the 20 year* study period. Additionally, these wells were located such that the region was surrounded on all sides, including the upgradient direction.

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- All of the wells located outside of the identified region of interest were used to determine the TDS "fingerprint" for the groundwater "background" conditions.
- Figure 1 shows the TDS star diagram for the determined background condition where 60 samples were available over the course of almost 20 years.

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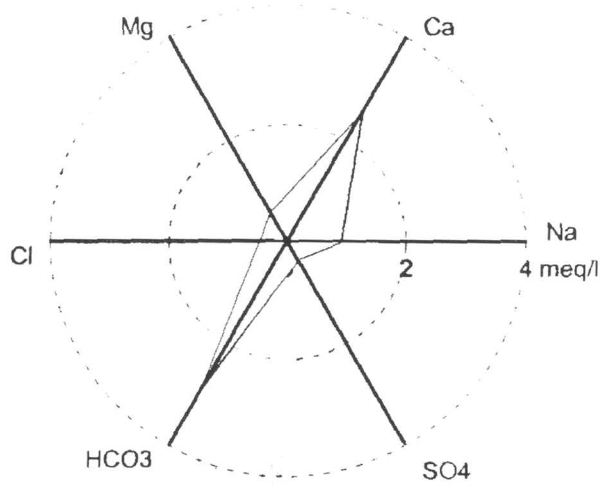
Figure 1. "BG" Star Diagram for "Background" Conditions (Weighted Average of 3 Background Wells, 60 samples)



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- Within the region, two samplings were available, at different times and locations, at the northeast upgradient area groundwater wells.
- These two wells had limited samplings available; therefore, the available sampling was used as "fingerprints", one for each well.

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- One well fingerprint, labeled X1 from well W-1, dated 1983, the other fingerprint, X2, from well W-2, dated 1998.
- These two fingerprints were assumed to be a representative mean value vector at the sampled locations because similar characteristics were observed in the sampled groundwater wells located downgradient.
- Thus, these two fingerprints, along with the background fingerprint ("BG"), are further examined in explaining all other downgradient well sampling measurements.
- Figures 2 and 3 show these other two fingerprints from wells W-1 and W-2. These fingerprints were called 2STAR and 3STAR, respectively.

Figure 2. "2STAR" Diagram, from Well W-2, in 1998

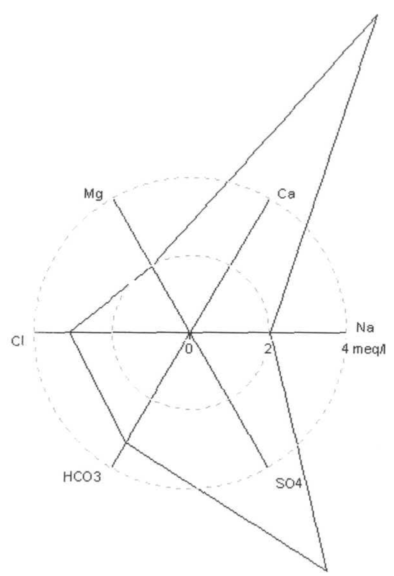

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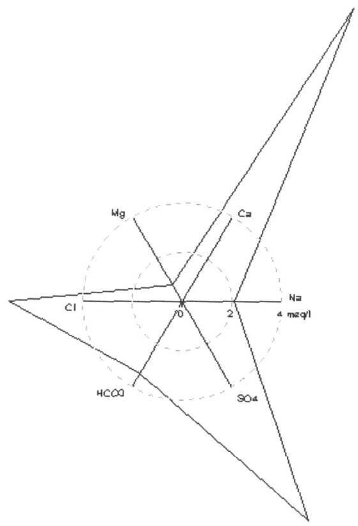
Figure 3. "3STAR" Diagram, from Well W-1, in 1983



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- Because of the groundwater flow field, these three fingerprints would need to be considered in the examination of well samplings taken downgradient.

- Both 2STAR and 3STAR are taken from wells located immediately downgradient of reported liquid waste disposal ponds, and are in close vicinity of each other, allowing for the possibility of mixing.

- Although only single point-in-time samples of 2STAR and 3STAR are available, they would be considered more of a time average measurement because of the storage of previous TDS inputs within the vertical soil column, above the groundwater.

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- Nonetheless, substantial information is contained in 2STAR and 3STAR, they both differ significantly from BG, and 2STAR and 3STAR show substantial similarity even though they are sampled at different wells and are separated by 15 years in time.

- In order to analyze the other well samplings and to investigate the explanation of these other readings using only BG, 2STAR, and 3STAR, a computer program was developed that determined the mixing proportions for each sample, using the underpinnings of a Hilbert Space setting.

❑ Hilbert Space Setting

- The three fingerprints considered, {BG, 2STAR, 3STAR}, are each composed of six TDS constituents of <Cl, HCO3, Mg, Na, SO4, Ca>.

- The numeric measurements of these constituents provide the components of a 6-dimensional vector. Thus, the three fingerprints can be represented as three 6-dimensional vectors, noted as v_1 for BG, v_2 for 2STAR and v_3 for 3STAR.

- Let S be the set of all 6-dimensional vectors. Then each of v_1, v_2, and v_3 are elements in S. Let W be the subspace of S spanned by v_1, v_2, v_3 where, for any v in W,

$$v = av_1 + bv_2 + cv_3$$

Eq. 1

where a, b, c are constants uniquely associated with the choice of v in W.

- It is also noted that only vectors with non-negative components are eligible to be considered in the water quality analysis.

- The vectors v_1, v_2, v_3 are said to be the basis of W.

- Each of the 214 groundwater samplings can be written as a dimension 6 vector and is an element of S.

- Let v_s be such a good sample. If v_s is a mixture of v_1, v_2, v_3, then there are values for the constants a, b, c, that satisfy Eq. (1), all constants being non-negative (constraints of the system), and therefore v_s is in W.

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- To determine the mixing proportion values of a, b, c, in Eq. (1), corresponding to a sampling vector v_s, a least squares minimization is achieved of the quantity X, where X is given by the usual ℓ_2 norm (Hromadka and Whitley, 1993).

- The minimization of X is achieved by a Gramm-Schmidt procedure, which is equivalent to finding the values of a, b, c that minimize the least squares difference between the above vector components.

❑ Modeling Results

- Each of the 214 samples were analyzed with respect to Eq. (2), resulting in 214 sets, of 3-element mixing proportions.

- By plotting the star diagrams, for each sample, and superimposing the star diagram developed by use of the mixing results from only the three fingerprints of {BG, 2STAR, 3STAR}, it was seen that the sampled data was substantially explained by using only the three fingerprints.

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- That is, there were few instances where the sampled data star diagram did not closely match the two contaminated fingerprints mixed with background groundwater.

- Figure 4 shows a few comparisons by superimposing star diagrams.

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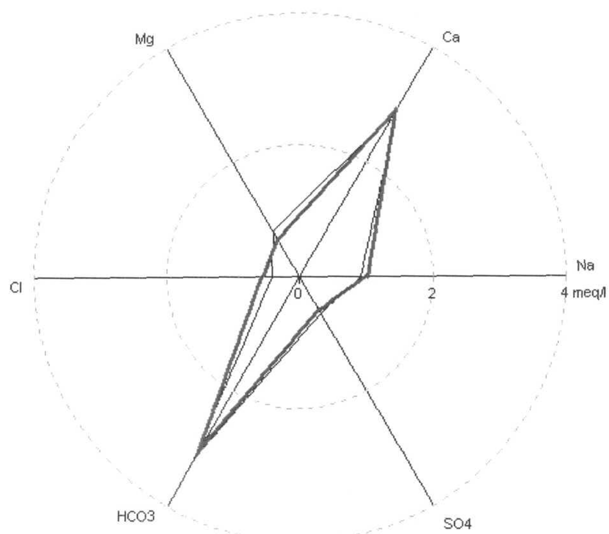
Figure 4. Hilbert-Space Approximation Results versus Measure Data, for subject Monitoring Well in 1989



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❑ Evaluation of Modeling Results

- The meaning of the modeling results is that the vast majority of groundwater well samplings, taken at many locations, and across some 20 years in time, can be explained by only mixing background water with two isolated fingerprints sampled within the interior of an industrial concern.
- These results are consistent with the groundwater flow trends, and the fact that these two isolated fingerprints were indeed caused by an event located at the most upgradient reaches of the small region under study.

- Mathematically, there is additional meaning to these results. The background BG vector is expected to be involved in any sample, any time.
- Therefore, the BG vector is really a commonality to the set of all possible samples, and hence can be viewed as not being a degree of variability in Eq. (1).
- That is, the departure from BG, for any sample, is what is under scrutiny, and is what is subject to availability.

- And yet this departure is well explained by only two vectors, 2STAR and 3STAR.

- Geometrically, one can visualize an analogy of this situation as being equivalent to 2 points (i.e., vectors) in 3-dimensional Euclidean space. The line *L* drawn through these two points is a depiction of the vector space spanned by the two given points.

- Of interest is that each groundwater samplings departure, from BG, plots to within a small distance from this conceptualized geometric line, but with that line in this case being plotted in 6-dimensional space.

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❑ Conclusions

- An interesting application of a Hilbert Space setting is to determine the mixing proportions of chemical fingerprints in explaining a wide variety of groundwater samples.
- A method to accomplish the apportionment of source contribution is to utilize the Hilbert space setting, where the determined chemical fingerprints are the basis vectors of a Hilbert space and the inner product is defined to be the usual vector dot product.

- The procedure is readily programmable and can be efficiently executed on a spreadsheet program for large quantities of sampling data.

For questions, please contact Dr. Ted Hromadka, (714) 241-0094 or ted@phdphdphd.com

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