Supplementary Material

The Diagenetic Fingerprint of Rotliegend Sandstones in the Groningen Gas Field

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Correspondence Analysis methodology

This appendix provides additional details regarding the application of Correspondence Analysis (CA) to the point count data of authigenic minerals, following the theoretical framework outlined by Greenacre (2017) and Rosera and Coleman (2021). The analysis is based on a contingency table where the rows represent different mineral species, while the columns correspond to individual samples. This tabulation forms an $i \times j$ matrix, N, where i denotes the number of mineral species and j represents the number of samples. To facilitate the analysis, this matrix is converted into a correspondence matrix, defined as:

$$P = \frac{N}{n}$$

where P is the correspondence matrix and n is the grand total, calculated as:

$$n = \sum_i \sum_j n_{ij}$$

The application of CA is based on an eigenvalue decomposition of a χ^2-distance matrix derived from the contingency table. This method identifies associations between mineralogical compositions and wells by measuring deviations from expected values under the assumption of statistical independence. The row (r) and column (c) masses, representing marginal probabilities, are first computed as:

$$r_i = \sum_j p_{ij}$$

$$c_j = \sum_i p_{ij}$$

These vectors, r and c, express the relative frequencies of mineral species and their occurrence across samples, respectively. The expected frequencies for each element in the original matrix are given by the product of these two vectors, while the elements of P represent the observed frequencies. The χ^2 statistic is then used to quantify deviations between observed and expected values, computed as:

$$\chi^2 = \sum_{i=1}^{I} \sum_{j=1}^{J} \frac{(p_{ij} - r_i c_j)^2}{r_i c_j}$$

CA aims to measure the similarity between mineralogical compositions across samples by computing a cross-product of two χ^2-distances for column variables j and k, expressed as:

$$\chi^2_{distance} = \sum_{i=1}^{I} \left(\frac{(p_{ij} - r_i c_j)}{\sqrt{r_i c_j}} \right) \left(\frac{(p_{ik} - r_i c_k)}{\sqrt{r_i c_k}} \right)$$

These values are computed for all column pairs, resulting in a table of standardized residuals. The resultant matrix, S, is then decomposed using singular value decomposition (SVD):

$$S = D_r^{-\frac{1}{2}}(P - rc^T)D_c^{-\frac{1}{2}}$$

where D_r and D_c are diagonal matrices containing the row and column masses, respectively. The decomposition follows:

$$S = UD_aV^T$$

Where U and V are orthonormal matrices, and D_a is a diagonal matrix containing singular values in decreasing order. The principal coordinates of rows and columns are then determined as:

$$F = D_r^{-\frac{1}{2}}UD_a$$

$$G = D_c^{-\frac{1}{2}}VD_a$$

The columns of matrices F and G correspond to decreasing singular values, with the first column representing the axis that explains the highest proportion of variance in the dataset. Since the original matrix is scaled by the grand total nnn, the relationships between rows and columns remain preserved, facilitating the interpretation of mineralogical trends. The singular values from D_a can be converted into principal inertias:

$$\kappa_k = \alpha_k^2, \;\; k = 1, 2$$

where K is the minimum of $(I - 1)$ and $(J - 1)$. The proportion of variance explained by the first axis is computed as:

$$\text{\% inertia of CA 1} = 100 \times \frac{\kappa_1}{\sum_k \kappa_k}$$

Additionally, the contribution of each mineral species or sample to a given CA axis can be determined, providing insight into which variables most strongly influence the differentiation observed in the ordination space. The contribution of the jth column to the kth axis is given by:

$$\text{Contribution of column } j = \frac{c_j g_k^2}{\kappa_k}$$

By applying this approach, Correspondence Analysis enables the identification of mineralogical patterns between wells, revealing associations that may be linked to depositional environment, reservoir structure, or burial history. The interpretation of the results follows from the positioning of samples and minerals in the CA ordination space, where proximities indicate mineralogical affinities and clustering tendencies.

Supplementary Figure 1

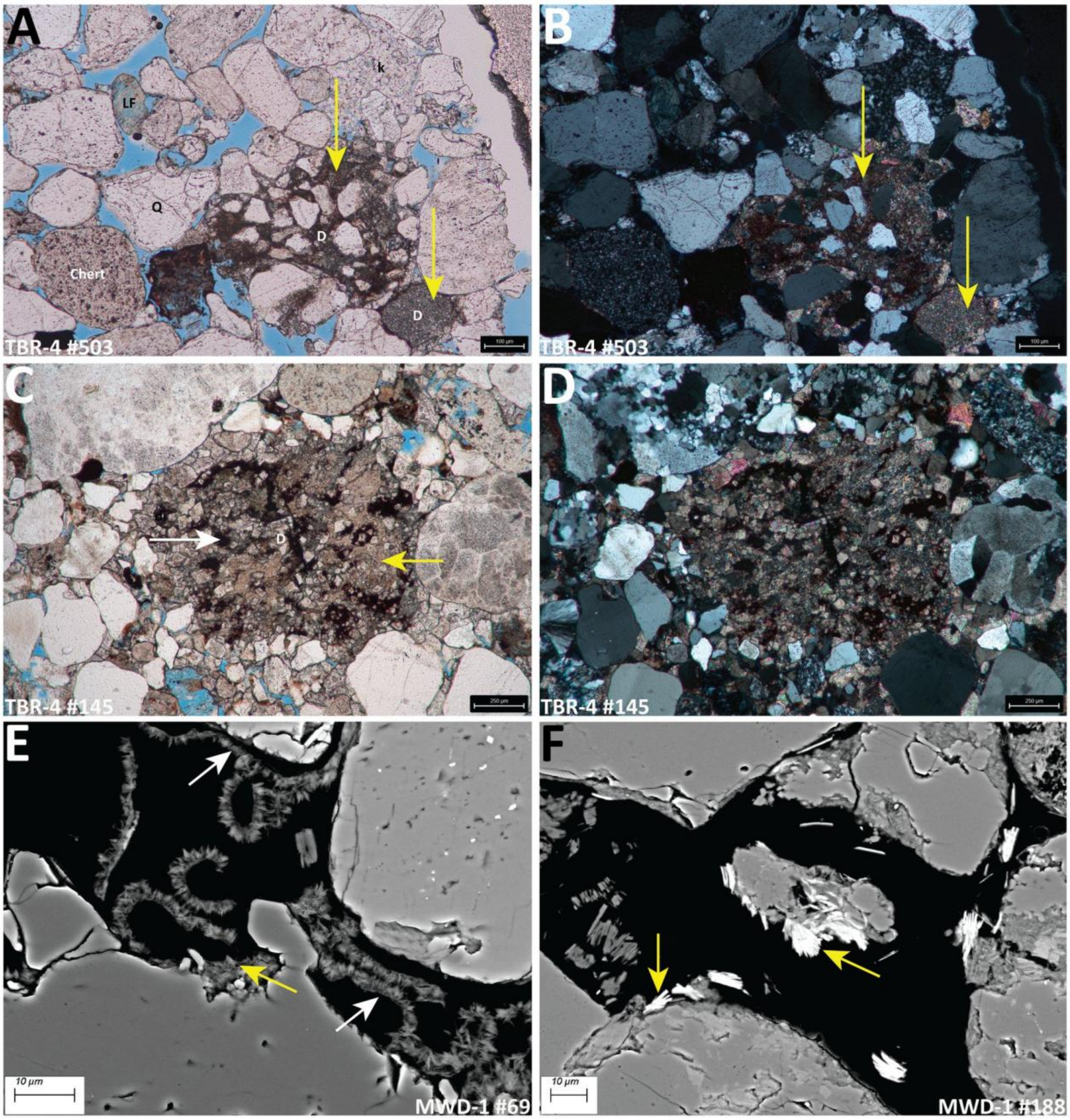

Figure S1: Different types of detrital carbonate intraclasts, detached radial illite, and chlorite rosettes. A-B) Plane and cross polarized light images of a detrital siliciclastic dolomite intraclasts (D) and a detrital carbonate intraclast with Fe-dolomite rim (yellow arrows). C-D) Plane and cross polarized light images of a detrital dolomite intraclast in which dolomite rhombs partially float in detrital clay. E) Radial illite that has been detached from the grain boundaries (white arrows). In one location the radial illite formed on an inherited clay cutan (yellow arrow). F) Fan-like arrangement of chlorite platelets on tangential illite and quartz grains (yellow arrows).

Supplementary Figure 2

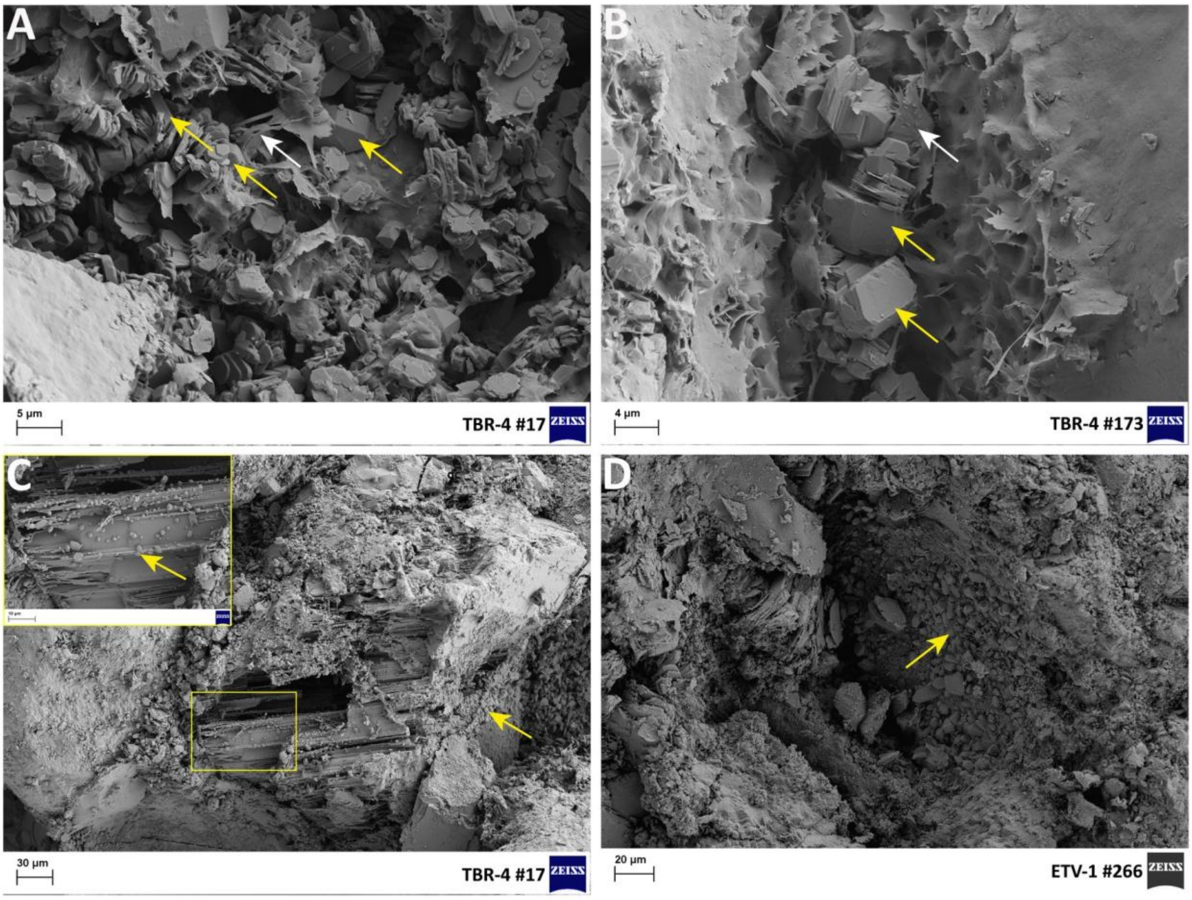

Figure S2: Kaolinite/dickite and microquartz in Rotliegend sandstones. A) SEM image showing kaolinite and dickite (yellow arrow) filling the pores where it is intertwined with fibrous illite (white arrow). B). Blocky dickite crystals in a narrow pore between two detrital grains. The radial illite covers the surface of the grains growing into the blocky dickite. C) SEM image showing microquartz that formed in and on a dissolved feldspar (yellow arrows). D) Microquartz on the intragranular surface of a dissolved grain.

Supplementary Figure 3

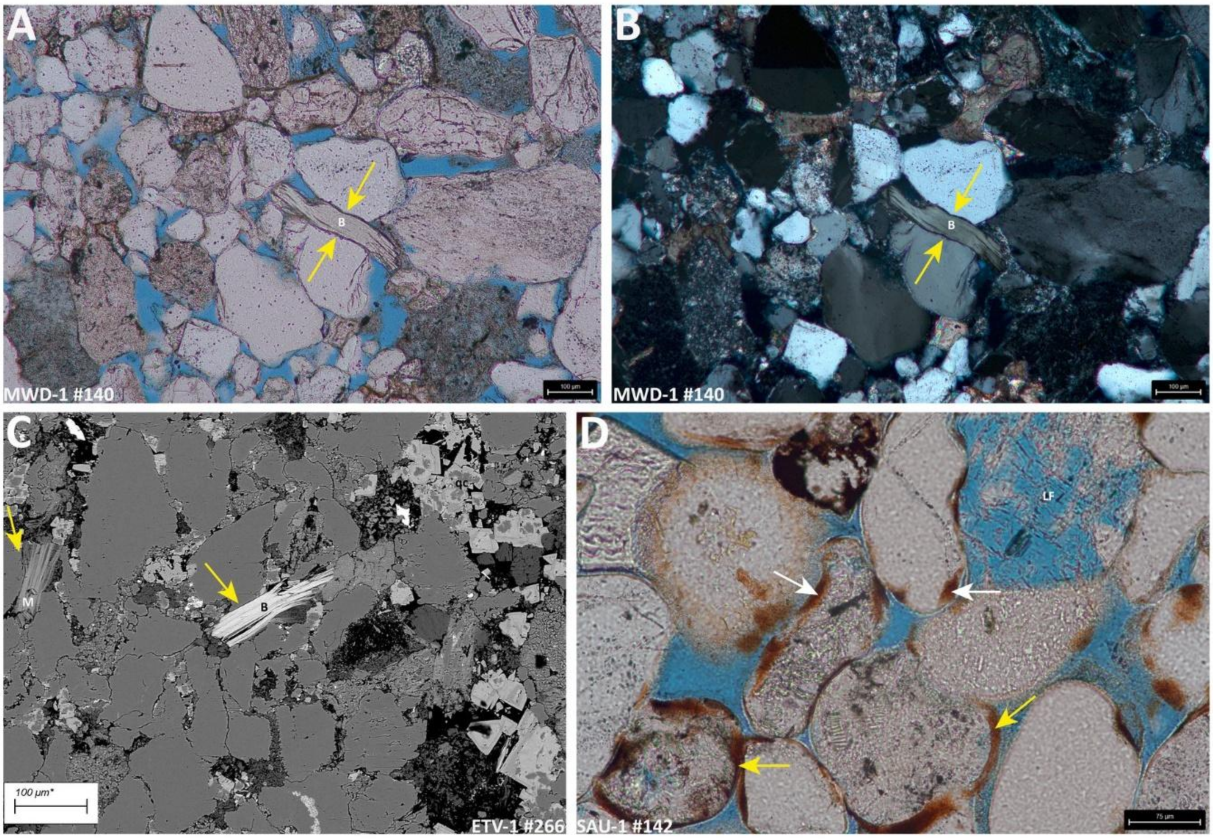

Figure S3: Pressure solution of quartz grains by mica and clay cutans in Slochteren sandstones. A-B) Plane and cross polarized light images that show pressure solution of quartz grains (yellow arrows) by biotite (B). C) SEM image that show pressure solution of quartz grains (yellow arrows) by biotite and muscovite (M). D) Slochteren sandstone from the aquifer well Sauwerd-1 (SAU-1) that contains grain enveloping clay cutans (yellow arrows) from soil infiltration and inherited clay cutans (white arrows) that were abraded during reworking of the sediment.