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A Tool for Thermo-sensitive Tracer Selection and Evaluation in Field Experiments

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ABSTRACT

The proper knowledge of the reservoir temperature distribution and precise prediction of the thermal breakthrough is essential for efficient energy yield and sustainable reservoir management. Recently, a number of hydrolyzable compounds with different kinetic properties, i.e., esters and amides, were proposed as thermo-sensitive tracers (TSTs) for characterizing the thermal state of geothermal reservoirs. Despite their coverage of wide ranges of temperatures and residence times, the practical application is still limited to lab scale. The required set of Arrhenius parameters for different compound classes is available from previous studies, but there is still no dimensioning tool that allows the characterization and evaluation of the tracer behavior at larger scale. In order to conduct a successful field tracer test, a comprehensive reservoir model, which is able to capture the tracer reaction and its compound-specific sensitivity for different temperature settings and residence time distributions (e.g., due to aquifer heterogeneities) is needed. In this study, a very flexible numerical tracer transport model is introduced that supports the tracer selection as well as the dimensioning and optimization of the test setup according to the prevailing reservoir conditions. The model results and limitations of thermo-sensitive tracers are presented for selected cases of high practical relevance.

1. INTRODUCTION

Against the background of climate change, there is an increasing focus in industrialized countries on the economically viable use of renewable energies (IPCC, 2011). Especially, geothermal energy is considered as an indispensable pillar in the energy mix of the future as it represents one of the largest renewable energy sources and it is further suitable for base load supply. The efficient and sustainable exploitation of the subsurface heat is crucial for the successful long-term operation of geothermal power plants. A common reservoir management strategy to enhance the extraction efficiency is the reinjection of geothermal fluids. However, this practice inevitably leads to a thermal drawdown in the injection region of the exploited reservoir and bears a potential risk of early thermal breakthrough in the abstraction well. This is because the extracted heat usually exceeds the natural heat flow in the subsurface (O'Sullivan et al., 2010).

Consequently, the proper knowledge of the reservoir temperature distribution and the precise prediction of the thermal breakthrough are essential components for a sustainable reservoir management and efficiency improvements in the geothermal power generation. In this context, a number of hydrolyzable compounds with different kinetic properties, i.e., esters and amides (Robinson et al., 1984; Robinson and Tester, 1990; Nottebohm et al., 2012; Maier et al., 2015a; 2015b; Schaffer et al., 2016), were recently proposed as thermo-sensitive tracers (TSTs) for characterizing the thermal state of geothermal reservoirs. However, their practical application is still limited to lab scale. Beside financial and technical constraints, the tracer application in the field also lacks from suitable dimensioning and tracer selection tools as well as comprehensive evaluation methods. Even though the Arrhenius parameters, which characterize the temperature-dependent tracer reaction, can be found for many compounds in the literature, there is no universal simulation tool available, which is able to model and analyze the tracer behavior for complex geometries and temperature distributions as encountered in potential and exploited geothermal reservoirs.

To close this gap and to foster the practical application of TSTs, a flexible reservoir transport modeling tool was developed. The tool is able to capture the reaction of several simultaneously applied tracer compounds and their evolution in the reservoir for different temperature settings (e.g., sharp/smooth thermal fronts) and flow conditions (e.g., different aquifer heterogeneities, hydraulic operation modes). In the presented study, several selected test cases were simulated and compared against a reference case in order to gain a deeper insight into the compound-specific tracer behavior and the sensitivity of relevant reaction and transport parameters. Furthermore, the additional benefit together with possible limitations of the parallel application of two TSTs are evaluated and critically discussed. Eventually, the presented model is an important contribution to the ongoing research on TSTs for reservoir characterization as it supports the tracer selection and, thus, the dimensioning/optimization of future field tests according to the prevailing reservoir conditions.

2. METHODS

2.1 Mathematical Model

The reactive transport of TSTs is described with a set of coupled partial differential equations. The main components of the model are the groundwater flow equation and the tracer transport equation. The governing equation for groundwater flow in porous medium is given as:

$$\frac{\partial}{\partial t}(\rho\varphi) - Q_i = \nabla \cdot (\rho \mathbf{u}) \tag{1}$$

where t is the time, ρ the fluid density, φ the porosity, Q_i a source/sink term, and $\boldsymbol{u}$ the Darcy velocity vector. The transport of the tracers follows the following advection-dispersion-reaction equation:

$$\frac{\partial c_i}{\partial t} = \nabla \cdot (D\nabla c_i) - \frac{\mathbf{u}}{\varphi} \cdot \nabla c_i + R_i \tag{2}$$

where c_i is the tracer concentration, D the dispersion coefficient, and R_i a reactive sink/source term for tracer compounds. The thermal sensitivity is given by pseudo-first order hydrolysis reaction in Eq. (3) for the TSTs and conservative tracer, respectively.

$$R_i = \begin{cases} -kc_i & \text{for} \quad TST \\ 0 & \quad conservative\ tracer \end{cases} \tag{3}$$

In Eq. (3), k is the first-order reaction rate constant of TSTs determined by the Arrhenius' Law:

$$k = Ae^{-\frac{E_a}{RT}} \tag{4}$$

where A is the pre-exponential factor, E_a the activation energy, R the ideal gas constant, and T the temperature.

In the following investigations, a two-dimensional vertical cross section (*xz*-plane) representing a reservoir area was setup. Further, a porous unconsolidated aquifer (no fractures) was assumed as modeling domain at this initial stage in order to focus on the general tracer behavior and effects before increasing the model complexity.

2.2 Model Case Description

2.2.1 Reference Case

The reference model is a simple case with uniform flow in a homogenous porous medium (10×2 m) under isothermal heat conditions. A constant temperature (T) of 100°C (373.15 K) is applied for the whole domain. A TST (1 g/L) was continuously injected with a constant injection rate of 10 L/s from the injection well (left side in Fig. 1) and the concentration of the reaction product was monitored in the production well (right side in Fig. 1). As internal reference, the same concentration of a conservative tracer was simultaneously injected together with the TST. The reference case intends to transfer the developed lab experimental setup to field scale, and therefore, the chemical properties of phenol acetate (Nottebohm et al., 2012; Maier et al., 2015a) were used for the TST.

2.2.2 Test Case 1– Heterogeneous Flow

Performing and analyzing tracer tests in the field is an important challenge, especially in reservoirs/aquifers with complex geometry. The groundwater velocity field, which is controlled by the heterogeneity of hydraulic properties, is the driving mechanism for alteration of the tracer breakthrough curves. To test the influence of aquifer heterogeneity on tracer transport (including conservative tracers and TSTs), the model domain was separated equally into two layers, an upper permeable layer and a lower less permeable layer. A scalar value (neglecting anisotropy of each layer) for the hydraulic conductivity of $K_{up} = 10 \cdot K_{low}$ was applied for upper and lower half of the model domain, respectively. Other parameters were equal to the reference case.

2.2.3 Test Case 2 – Linear Temperature Gradient (single TST test)

In general, according to Arrhenius Law, higher reservoir temperatures result in higher *k*-values and thus higher reaction rates of TST can be expected (Eq. 4). To test the influence of the temperature distribution of a reservoir on tracer transport and reaction a gradually decreasing T from 110°C to 90°C was applied along the 10 m long *x*-axis and the same average temperature was kept than the reference case (T_{ave} = 100°C). Due to the non-linear dependency of k on temperature, a higher *k*-value is expected.

2.2.4 Test Case 3 – Non-linear Temperature Gradients (multiple TST test)

In the field, the water temperature in the injection well and production well can directly be measured. Hence, the temperature range of the thermal gradient between the two wells is known. However, the spatial (and temporal) distribution of the temperatures between the injection and production wells is usually unknown. The two block model presented by Maier et al. (2015b) characterizes the temperature distribution discretely by means of a cooled fraction (one cold and one hot zone). Consequently, the hypothetical position of an assumed abrupt thermal front and the mean temperature of the geothermal field can be calculated. As this method assumes an unrealistic sharp separation of the temperature field, its practical application as an indicator for thermal breakthrough is limited (too late). The formation of smoother thermal fronts and, thus, earlier arrivals of the thermal breakthrough seem to be more realistic.

In the presented model, the shape of the thermal front and, consequently, the temperature distribution of the domain between the two wells, is assumed to be smooth and thus more realistically described by the shape of a symmetrical sigmoid function. Therefore, the following expression was applied (scaling the error-function to the domain):

$$T(x) = T_{in} + \Delta T \cdot (erf(\beta \cdot (x - x_{center}) + 1) / 2 \tag{5}$$

where T_{in} is the temperature in the injection well, ΔT the temperature difference between the injection and the production well, β a smoothing factor characterizing the steepness of the thermal front, x_{center} the position of the thermal front (center of gravity). In this case, x_{center} was set in the middle of the two wells.

To gain an overview over the influence of different front shapes on TST transport, β was varied in the range of 0.5 to 5. Note that the sharper the thermal front, the higher is the value of the smoothing factor (see Fig. 1). In order to test the sensitivity of TST behavior from β, three TSTs with different kinetic properties (tracer selection see section 2.3) were simulated. Furthermore, ΔT and the tracer residence time (t_{res}) were varied for each respective case.

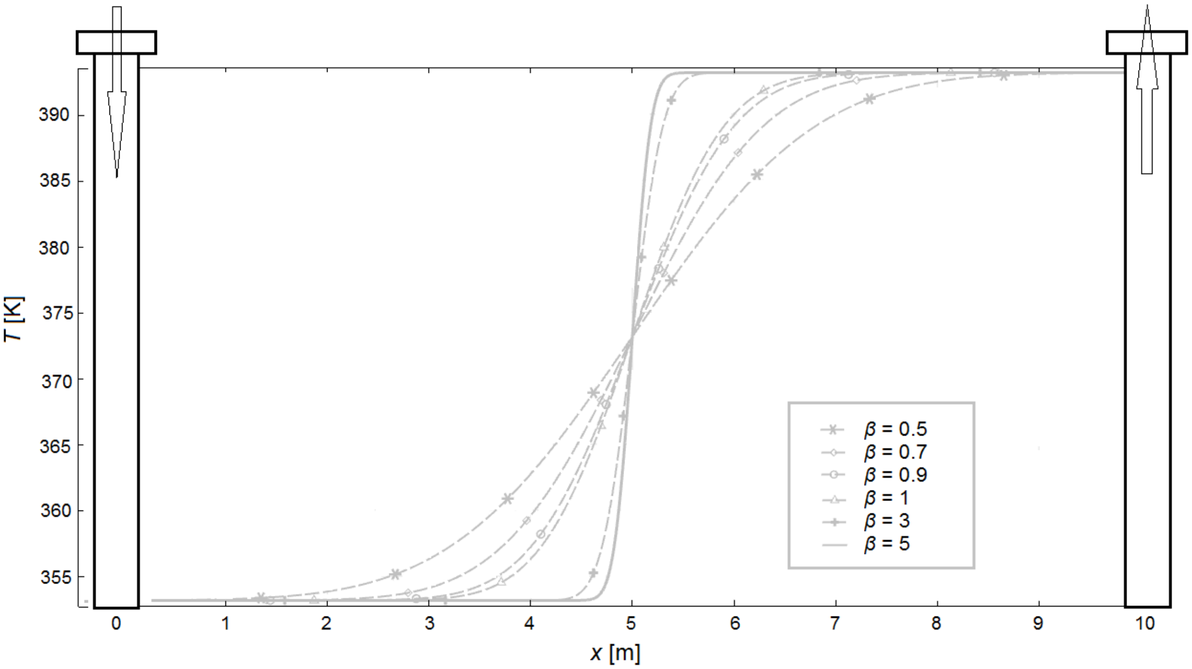

Figure 1: Principal sketch of the model set-up and the temperature distribution of the reservoir for different shapes of the thermal front.

In contrast to case 1 and 2, where the conservative tracer and TSTs are continuously injected into the reservoir, a pulse injection (1 g/L for 1 min) was applied in this case (case 3).

2.3 Thermo-sensitive Tracer Selection - Arrhenius parameters of available tracer molecules

Since the idea of using thermos-sensitive tracers for estimating the thermal state of a reservoir is introduced, a number of chemical compounds with different reaction kinetics were proposed for different temperature conditions. Fig. 2 summarizes the E_a and ln A values of the potential TSTs proposed in the literature (Nottebohm et al., 2012; Robinson and Tester 1990; Schaffer et al., 2016). Despite an expected compensation effect (Plummer et al., 2010), different E_a to ln A ratios between 2 and 5 can be achieved. In the tested case (case 3), ln A was set to 25 1/h and typical E_a to ln A ratios between 2.9 and 3.3 (2.9, 3.1, and 3.3) were applied, where the majority of the tracers can be found (mostly esters).

3. RESULTS AND DISCUSSION

3.1 Influence of flow heterogeneity

The concentration of the conservative relative to the reactive tracers (TST_m = mother compound, TST_p = daughter compound (products)) are compared for homogenous flow (reference case) and heterogeneous flow, respectively (Fig. 3). Hydraulic conductivity generally influences the Darcy velocity and thus the transport velocity distribution (breakthrough curve shape) of the tracers. For the heterogeneous case the breakthrough curves become smoother and are associated with an earlier arrival and later (full) recovery of the tracer compounds. When comparing the decay of the same TST for both cases, it is obvious that the final concentrations are equal (plateau) for the same residence time and thus the amount of reacted tracer is constant. Furthermore, the breakthrough curves of both, the conservative and the TSTs, are equally influenced by the hydraulic heterogeneities. This implies for the tracer evaluation that flow heterogeneities (and dispersive effects) can be taken into account by evaluating the TSTs relative to the respective conservative tracer (ratio).

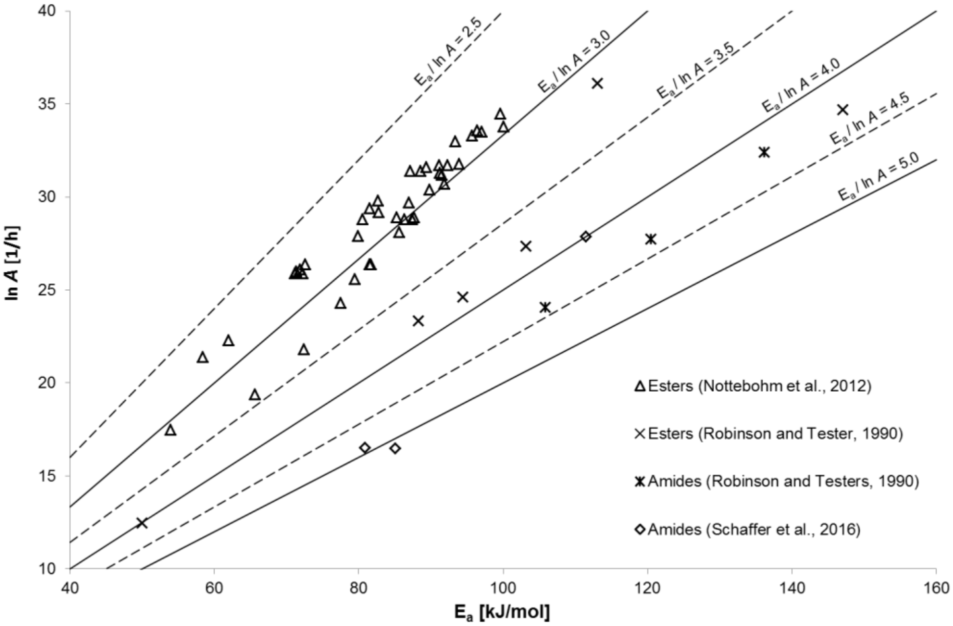

Figure 2: Available Arrhenius parameters and E_a to ln *A* ratios of TSTs from the literature.

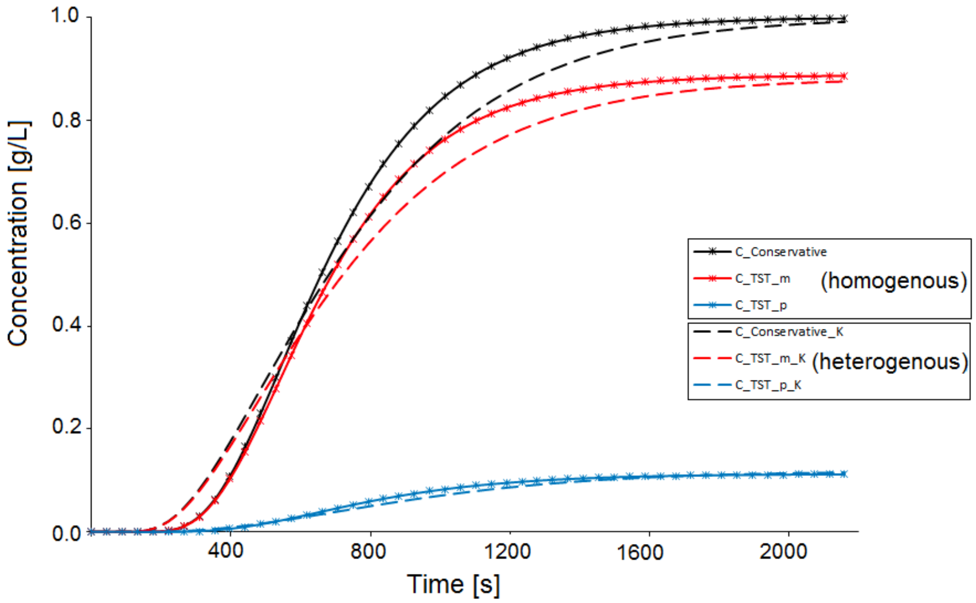

Figure 3: Comparison of tracer (conservative and TSTs) transport and reaction for homogenous and heterogeneous flow conditions.

3.2 Effect of Linear Temperature Gradient on Tracer Reaction (Single TST)

The breakthrough curves of the conservative and the TST for two different temperature settings are shown in Fig. 4. Logically, the shape of the conservative tracer (no reaction) is not influenced by the temperature. In contrast, the curves of the (same) TST and thus the effective reaction rates are different, even though the average temperature of the domain is equal. This behavior is expected (Maier et al., 2015b) and can be explained by the exponential increase of the reaction speed with increasing temperatures (see Arrhenius law, Eq. 4). This means that the tracer is reacting relatively faster at higher temperatures. Consequently, the tracer reaction is higher in the case of a linear temperature gradient, because higher absolute temperatures are reached. This is in accordance to Maier et al. (2015b) where the obtained values for the equivalent temperature in non-isothermal environments are shifted towards higher temperatures. These differences already imply a certain potential (sensitivity) of the TST reaction for the applied temperature field.

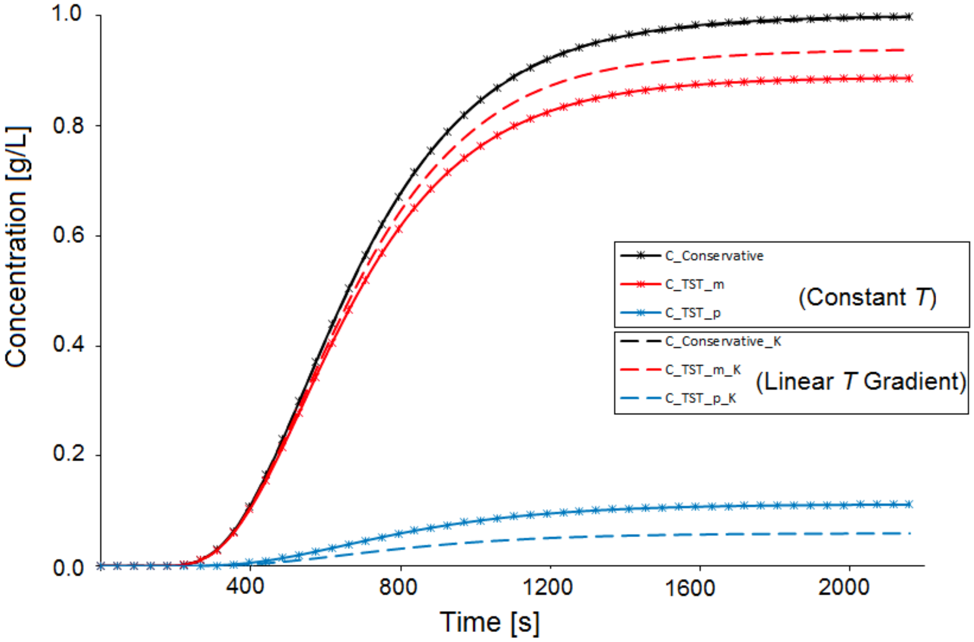

Figure 4: Comparison of tracer (conservative and TSTs) transport and reaction at the constant temperature and the linear temperature gradient condition (average temperature is equal)

3.3 Effect of Non-linear Temperature Gradients on Tracer Reaction (Multiple TSTs)

In order to test the tracer sensitivity with respect to the applied temperature field and to gain more information of the shape of the thermal front, the behavior of three simultaneously injected TSTs was investigated for different temperature distributions (same average temperature). As in the example before (Chapter 3.2), the obtained effective reaction rates of all three TSTs differ according to the applied thermal distribution. Generally, the TST having the lowest E_a (2.9·ln A) showed the fastest reaction and the tracer with the highest E_a (3.3·ln A) showed the slowest reaction for all applied gradients (ln A = *const.*). Based on each single TST, a mean temperature or cooling fraction can be determined based on a two block model (Maier et al., 2015b). In order get additional information on the shape of the thermal front, the ratios of the peak areas of two TSTs, initially normalized to the conservative reference tracer, were calculated (for every tracer combination) and correlated with the smoothing factor β (Fig. 5). As can be seen in Fig. 5, the resulting TST peak area ratios are slightly differing, especially for smooth thermal fronts (low β). Consequently, the ratio of two tracers shows a sensitive behavior to the shape of the thermal front and can potentially be used to determine β from tracer tests. On the one hand, the differences of the ratios are still relatively small, which impedes a reliable tracer evaluation. On the other hand, the sensitivity increases with higher temperature gradients. The results further indicate that the ratio change also depends on the selected tracer set used for the evaluation. According to the applied temperature conditions, different sets of tracers showed different sensitivities to β. The obtained absolute values for the tracer peak area ratios are a function of the residence time and, therefore, have to be individually determined for each case (hydraulic conditions).

4. OUTLOOK

In future investigations, the general influence/sensitivity of more relevant transport parameters on the tracer reaction has to be studied in order to understand/exploit the full potential of TSTs for reservoir characterization. Further optimization of the tracer selection is in progress (finding the optimal set of (at least) two TSTs) in order to achieve the highest possible sensitivity for describing the steepness of the thermal front in the reservoir according to the prevailing temperature conditions. Generally, the application and investigation of different mathematical functions to describe the front shape is conceivable. In order to further increase the flexibility and thus applicability of the modeling tool for field studies, the model is planned to be extended to account also for fracture flow. However, this will be done after the tracer behavior is fully understood. Eventually, the temperature distribution is believed to be reconstructed based on multiple TST tests. In the first step, a two block model is applied to localize the center of the thermal front by simply relating each TST to the conservative tracer. In the second step, the direct comparison of (at least) two TSTs allows the determination of the steepness of the thermal front and, thus, is able to provide an early warning for thermal breakthrough when the same tracer tests are repeated at different times.

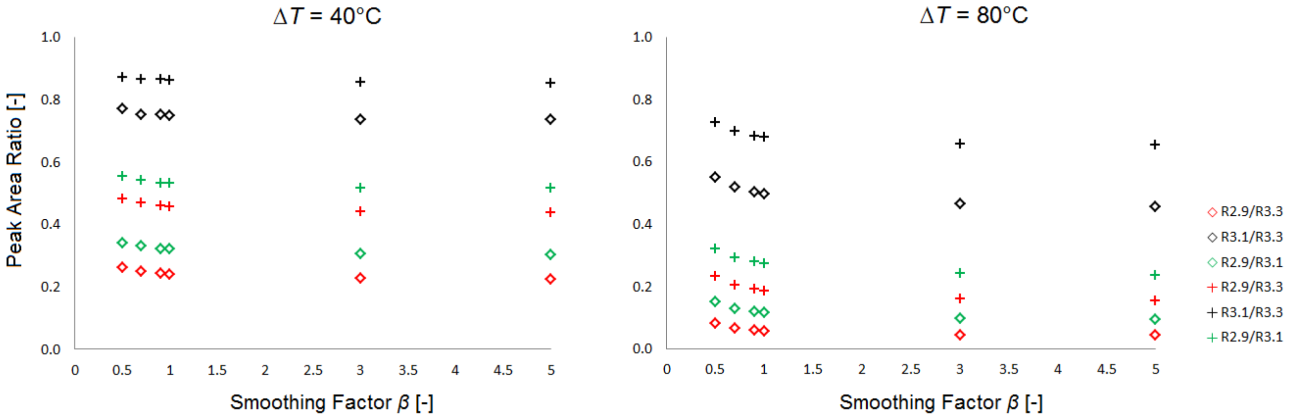

Figure 5: Change of the peak area ratios depending on the applied smoothing factors for two different temperature differences.

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