Void Evolution in Soluble Rocks: Development and Validation of Numerical Models by Field Evidence

Final report

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Summary

Karst aquifers are highly vulnerable to contamination due to the rapid transport of pollutants in conduits developed by the dissolution of rock. In addition, the presence of voids in the subsurface can cause severe engineering problems such as dam failure and land subsidence or collapses. The assessment of such environmental impact problems requires an adequate hydrogeological characterisation of karst terrains focusing on solution conduits and voids. Thus, this work aimed to improve our understanding of the interdependency between hydraulic and chemical processes involved in speleogenesis, and the geometry of the resulting cave patterns. Building on earlier research that focussed on *generic* conceptual settings, it was attempted to establish *site-related* models that are largely based on field observations but not intended to represent details of the evolution of specific caves. The study sites were located in the karst terrain of the Western Ukraine, as this area is well documented, displays the full sequence of karst evolutionary stages, and hosts a wide variety of karst phenomena.

To examine the interrelation between hydrogeological environment and conduit development in the deep-seated settings of the Western Ukraine, simplified model settings were designed based on an existing conceptual model. A coupled continuum-pipe flow model, representing the fractured porous rock by a continuum approach and the solution conduits by a discrete pipe network, was employed for simulating conduit development under various conditions. In agreement with field observations, the evolving cave patterns were found to be characterized by pronounced horizontal passages and multiple vertical conduits at the bottom of the soluble unit but only few at the top. The frequency distribution of conduit diameters was found to be bimodal if the permeability of the rock formation is sufficiently high to allow competitive conduit development governed by the feedback between increasing flow and dissolution rates. This feedback, however, is suppressed in low-permeability formations. As a consequence, conduit development was found to be uniform rather than competitive in the corresponding model scenarios. Our results further reveal effects of the spatial extension of the discharge area, the variability of initial apertures, and the chemical saturation of the water on cave patterns evolving. More generally, our results suggest that numerical modelling is not only useful for studying the general interactions of physical and chemical processes governing karst evolution. The translation of site-related conceptual models to numerical model scenarios can provide further insight into speleogenetic mechanisms and controlling factors of karst evolution in specific types of settings.

Final progress report

This study was proposed as a three-year project (with the third year to be approved following a renewal proposal) that included the Principle Investigator's (PI) own salary. As the PI was appointed to a professorship at the University of Graz (Austria) at the early stage of the project, the PI's position was replaced by that of a PhD student, thus involving the need to instruct a new employee. Moreover, the eligibility criteria for a renewal proposal were not met anymore such that the total duration of the project was reduced to two years. Consequently, the work schedule and the individual work packages had to be adapted. Nevertheless, the overall objectives of the project were achieved, as demonstrated by the summary provided by this report and the more detailed publications cited herein.

1. Objectives

Flow in karst aquifers is concentrated along solution conduits. Solution conduits develop where discontinuities are widened due to dissolution of rock. Together with the surrounding fractured porous rock, these conduits form a complex and heterogeneous flow system. About one quarter of the world's population is largely or entirely supplied by karst waters (Ford and Williams, 2007). These important groundwater resources are highly vulnerable to contamination due to the rapid transport of pollutants in the karst conduits. As well, the presence of voids in the subsurface can cause severe engineering problems such as dam failure and land subsidence or collapses. The assessment of such environmental impact problems requires an adequate hydrogeological characterisation of karst terrains focusing on conduits and voids developed by the dissolution of rock. One approach to tackle this challenge is to improve our understanding of the interdependency between hydraulic and chemical processes involved in speleogenesis, and the geometry of the resulting cave patterns.

The overall objective of the accomplished project was to improve the knowledge about the temporal and spatial evolution of karst aquifer void systems as a consequence of the hydrogeological environment, thus contributing to various applied topics such as those mentioned above (e.g., aquifer vulnerability, land subsidence or dam failure).

In order to examine subsurface void evolution in karst terrains, numerical models are increasingly applied. Since it has been considered as impossible to simulate the evolution of *specific* cave systems, earlier research focussed on *generic* conceptual settings. Attempting to reduce this gap with a view to substantiate conclusions on "environmental impact problems" (Ford and Williams, 2007) such as karst geohazards, this project aimed at establishing *site-related* models that are largely based on field data but are not intended to represent details of the evolution of specific caves.

2. Methods

Site-related numerical models of karst evolution rely on the development of conceptual models that are based on field observations from selected cave systems. Extensive field observations such as information about the genereal geological and hydrogeological setting, dissolution rates, recharge-discharge relationship, and fissure patterns were available from the gypsum karst of the Western Ukraine. Moreover, a conceptual model of speleogenesis was developed (Klimchouk, 1997, 2000a, 2000c, 2005) based on these observations and generalised to be applicable to many regions around the world (Klimchouk, 2007). Thus, the field observations and the related conceptual model of spelegenesis in the Western Ukraine was revisited and translated into numerical model scenarios in close collaboration with Dr. Alexander Klimchouk (Institute of Geological Science, National Academy of Science of Ukraine).

Using the numerical models, the conceptual model was tested and iteratively improved by comparing simulation results with field observations. Thereby, it was attempted to achieve general agreement, e.g., of the overall cave pattern rather than to reproduce field data exactly. The numerical model Carbonate Aquifer Void Evolution (CAVE), initially designed to simulate conduit development in limestone (Clemens et al., 1996; Liedl et al., 2003), was applied in this project. Conceptually, CAVE is a dual flow model, treating flow in the fractured porous rock as a continuous flow field (continuum model) and flow in the discrete and localised conduits (conduit model) as two interconnected flow systems, each characterised by its own hydraulic parameters and flow equations (e.g., Bauer et al., 2005; Birk et al.; 2003, Liedl et al.; 2003, Rehrl et al., 2008b).

3. Results

3.1 Conceptual Model

Figure 1 (upper part) illustrates a typical hydrogeologic profile across the gypsum belt in the present artesian zone depicting natural (pre-quarrying) conditions. It shows a realistic tectonic setting for cratonic edges bordered with foredeeps and is observable in the Western Ukraine (Klimchouk, 2007). A gypsum layer is sandwiched between less soluble porous/fissured formations. The gypsum layer is initially less permeable than the adjacent formations. Thus, the gypsum separates two aquifers in a confined flow system. The upper aquifer is formed by the lower part of the Kosovsky Formation (clays and marls with minor sandstone beds), the Ternopols'sky Beds (lithothamnion marly limestones), and the limestone bed of the Tyrassky Formation (pelitic marine and epigenetic limestones). The lower Badenian sandy carbonates, in places along with Carboniferous sediments, form the lower aquifer. Investigations by Klimchouk et al. (1995) and Klimchouk (1997, 2000a, 2000b) suggest that the hydraulic conductivity of the lower aquifer is typically higher than that of the upper aquifer. The gypsum units of the Western Ukraine are characterised by a pronounced vertical structural heterogeneity caused by the discordance of the fissure networks between different horizons. A typical three-dimensional pattern is depicted in Figure 2. More details about the conceptual model and the stratigraphic, lithologic, and structural characteristics of the study sites can be found in Rehrl et al. (2008b, 2009).

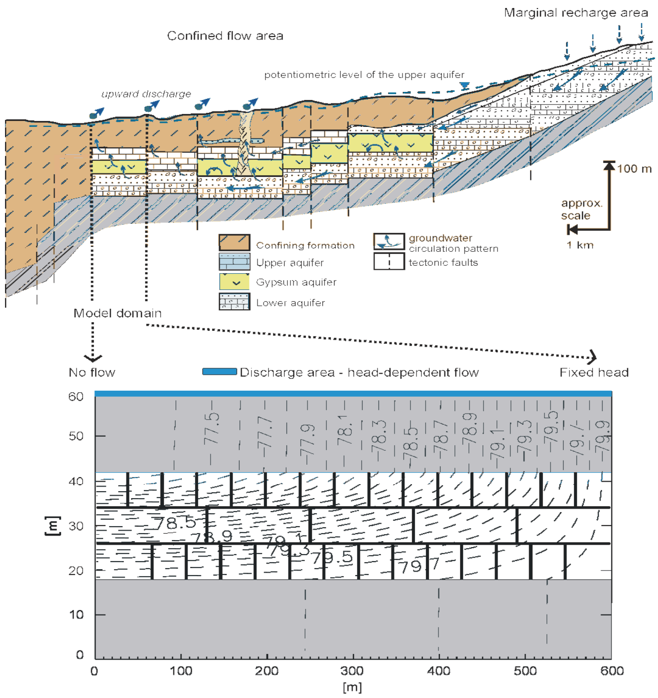

Figure 1: Conceptual model and circulation pattern of an artesian setting (upper part) and its integration into a numerical model (lower part). Litho- and hydrostratigraphy corresponds to the case of the Western Ukraine. The lower part shows the modelling domain including boundary conditions. The dashed lines represent the hydraulic heads in the fractured porous rock and the dark solid lines illustrate the network of protoconduits at the beginning of the simulation (from Rehrl et al., 2008b).

A simplified conceptual model was designed by Rehrl et al. (2008a) and later successively modified (Rehrl et al., 2008b, 2009) to examine the influence of various factors on conduit development within this type of setting. The complex three-dimensional structure depicted in Figure 2 was approximated by two-dimensional model scenarios (Fig. 1, bottom). Within this two-dimensional vertical cross-section, the actual three-dimensional structure of the fissure network is approximated. The recharge area is represented by a fixed hydraulic head at the right margin of the model, i.e. flow is from right to left. The bottom and the left hand side of the model domain are no-flow boundaries. Discharge is through the upper boundary, which is represented by a head-dependent boundary condition as described by Rehrl et al. (2008b). The outflow at this boundary depends on the hydraulic conductivity and the thickness of the confining bed covering the aquifer and on the elevation of the land surface, which is always below the hydraulic head in the aquifer system (artesian setting).

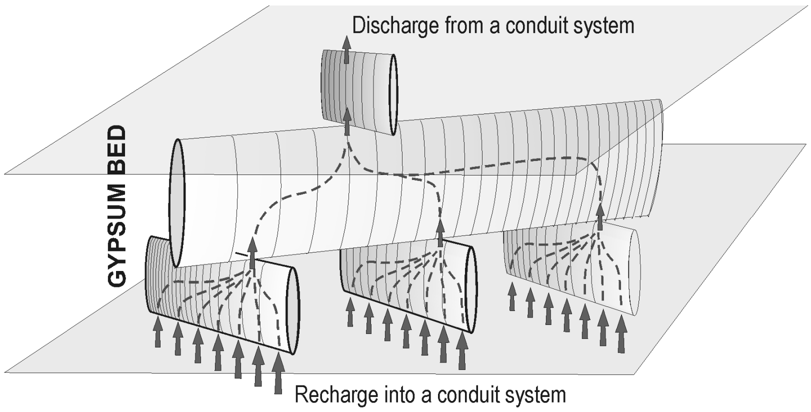

Figure 2: Vertical structural heterogeneity and transverse flow through fissure networks in multiple levels (from Klimchouk, 2007).

3.2 *Numerical simulations*

Rehrl et al. (2008a) considered the influence of the recharge/discharge relationship on the karstification process by variations of the extension of the head-dependent upper boundary. The initial apertures of the protoconduits were uniformly distributed at the beginning of the simulation. The results showed that the conduit evolution in a setting with a spatially localised discharge area is slowed down, especially in the upper part of the gypsum, and more restricted to the discharge area as opposed to settings with a spatially extended discharge area.

Rehrl et al. (2008b) additionally examined the influence of the hydraulic conductivity of the entire formation, which may vary over several orders of magnitude in the given lithological environment. In a first scenario (basic scenario) the hydraulic conductivities were adapted from Birk et al. (2003) (high hydraulic conductivity setting); in a second scenario the hydraulic conductivities of the entire rock formation were reduced by a factor of one hundred (low hydraulic conductivity setting). A third scenario considered the influence of the chemical saturation with respect to gypsum of the inflowing aqueous solution on the karstification process. While the gypsum layer was supplied with highly aggressive water in scenarios one and two, the water was assumed to be close to chemical saturation in the third scenario.

Figure 3 shows the conduit pattern developed in scenario one: Initially, the hydraulic head of the upper aquifer is significantly lower than that of the lower aquifer. Thus the protoconduits are supplied with solutionally aggressive water from below and the development of conduits following the upward directed hydraulic gradient. During the early stage of speleogenesis (200 years), illustrated in Figure 3a, the flow rates in the protoconduits are limited by the narrow outlets at the upper boundary of the gypsum bed. Because of the low flow rates the water approaches the switch concentration soon and thus the dissolution rates are low, following a higher-order dissolution kinetics. At the top of the soluble unit the protoconduits are not enlarged at the beginning due to the high saturation of the aqueous solution with respect to gypsum when it reaches the upper part of the conduit network. With ongoing simulation period, the widening of conduit apertures nevertheless increases the flow rates and thus the dissolution rates. At a later stage (500 years) water with a solute concentration below the switch concentration emerges at the outlet at the top of the soluble bed, such that the more efficient linear dissolution kinetics is active along the entire flow path. This situation is denoted as breakthrough (Fig. 3b) and intensifies the operative positive-feedback mechanism. This leads to a significant increase in discharge through the conduit system and solutional widening of conduit apertures. A more detailed description is provided by Rehrl et al. (2008b).

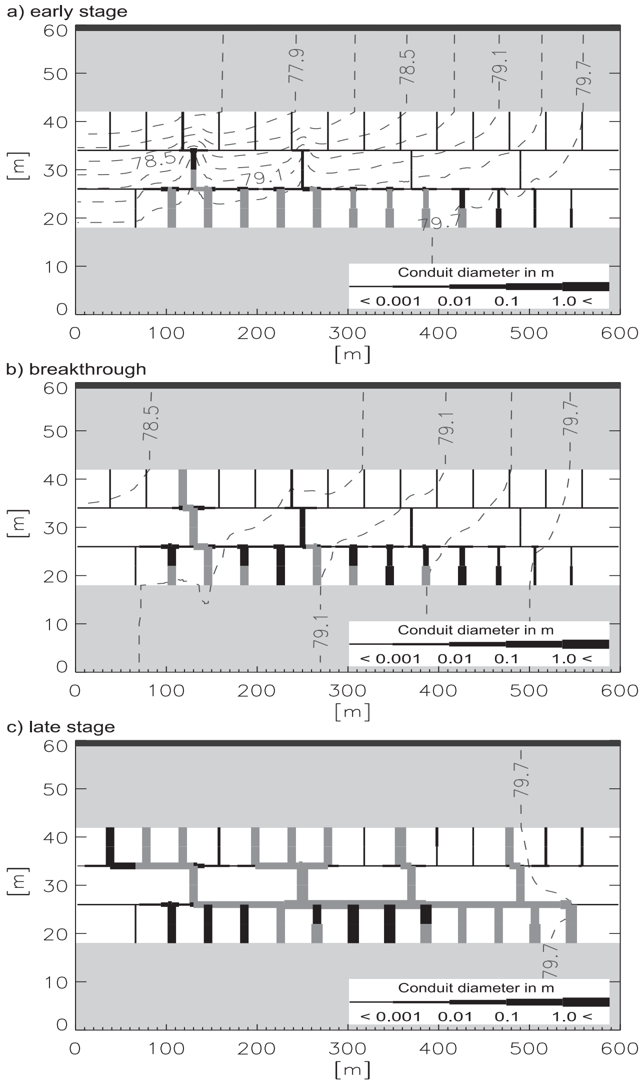

Figure 3: Computed conduit diameters and hydraulic heads (dashed lines) in the fractured porous rock (in m). The top shows the early stage (400 years), the middle illustrates the situation after breakthrough (500 years), and the bottom shows the late stage (10^4 years) of karstification. Gray shaded pipes indicate that the outflow concentration of the aqueous solution is less than 94% (switch concentration) saturated with respect to gypsum. The dark and thick drawn line at the upper edge of the model domain refers to the discharge area (from Rehrl et al., 2008b).

The breakthrough of a vertical pathway and the subsequent development of large-aperture conduits diminish the vertical hydraulic head difference between the lower and upper aquifer. However, in the case of a lateral extended discharge area a significant hydraulic gradient is still maintained, such that the evolutionary process proceeds from the left to the right side of the model domain. Because of the large apertures, at the late stage the hydraulic resistance of the well-developed conduit pathways is very low and the flow rates are limited by the permeability of the non-soluble aquifers and the boundary conditions of the flow system. At a late stage of conduit development (10^4 years, illustrated in Fig. 3c), flow and gypsum dissolution are focused to the conduits where the breakthrough has occurred. Thus the exchange of water between the network of conduits and the continuous flow system, which is important at the early stage of conduit development, becomes negligible. The hydraulic gradient between the two aquifers is reduced and the flow rate does not increase anymore. Thus flow rates through other conduits in the network are low and the evolution of these conduits proceeds only slowly.

Figure 4 shows the cumulative frequency distributions of the conduit diameters for several time steps. The solid lines denote the case of a laterally extended and the dashed lines that of a laterally localized discharge area. A bimodal aperture distribution is obtained. This can be attributed to the vertical breakthrough and the associated strong feedback mechanism. If the concentration drops below the switch concentration the first-order dissolution kinetics is effective and solutional widening of the conduits becomes faster. Hence a certain range of apertures is not well pronounced. This means that the already enlarged conduits continue to increase and the remaining conduits stay small-sized. In the case of a localized discharge area the evolution is slower. However, after a long time period the cumulative frequency distribution approaches that of the scenario with the extended discharge area. The results by Rehrl et al. (2008b) thus show that the structure of the mature conduit system is not finally determined during the early stage of karstification as suggested by Birk et al. (2003). If karstification proceeds over long time periods under constant boundary conditions, differences in early conduit patterns resulting from different discharge modes may be overridden in the long-term. Nevertheless, such different discharge modes might be a controlling factor in conduit development under changing environmental conditions.

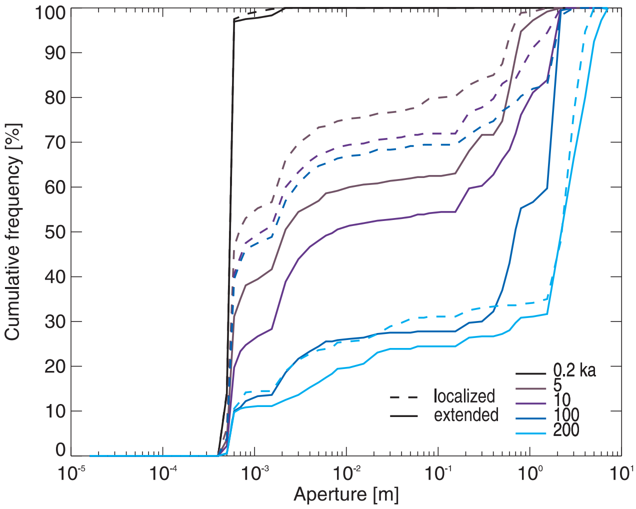

Figure 4: Time dependent cumulative percentage of conduit aperture data at different times and scenarios with different upper boundary conditions. The solid lines correspond to a laterally extended and the dashed lines to a localised discharge area. Black lines denote the early stage (200 years) and the colored lines denote the later stages ($5x10^3$ years and 10^4 years) of karstification. Also long time simulations (10^5 years and $2x10^5$ years) are plotted (from Rehrl et al., 2008b).

Contrary to the basic scenario the cumulative frequency distribution of the conduit apertures is not bimodal in scenario two, where the hydraulic conductivities of all units were reduced by a factor of one hundred compared to the basic scenario. Because of the suppressed flow breakthrough events involving first-order dissolution kinetics along an entire flow path are very rare and temporary. Hence the pronounced feedback mechanism arising from such events is not operating here, i.e. conduit development is less competitive. As a result there is a smooth transition from nearly undeveloped protoconduits to well developed conduits rather than a clear and distinct separation. With ongoing simulation time more and more conduits evolve, but the growth rate is small due to the low flow rates. Contrary to the basic scenario, the frequency distribution obtained at an early stage remains almost unchanged during the entire long-term simulation. Thus the entire network of protoconduits is uniformly widened at a low rate. Conduit pattern and aperture frequency distributions are similar for both extended and localized discharge (Rehrl et al. 2008b).

In deep-seated, layered aquifer systems, the soluble units are fed by waters from adjacent soluble or non-soluble units, which may exhibit highly variable solute concentrations of the inflowing aqueous solution (e.g., Klimchouk and Aksem, 2005). In fact, the water can be close to saturation when it enters the network of protoconduits. This situation is examined in scenario three. Rehrl et al. (2008b) demonstrated that in this case the temporal evolution of the conduit aperture distribution yields a bimodal structure that is less pronounced than that in the basic scenario. The karstification process is very slow due to the high chemical saturation of the water flowing into the conduit system. Even after a long time only few conduits with an aperture >1 m evolve, while most of the conduits stay in the order of a few decimetres. Thus similar to the low-permeability scenario conduit development appears to be less competitive than in the basic scenario.

Rehrl et al. (2009) examined the influence of random aperture variability on dissolutional growth of conduits in hypogene settings thus extending the work by Rehrl et al. (2008a, b). This kind of random heterogeneity was represented by employing a second-order Gaussian random distribution of initial aperture data within the network of protoconduits, i.e. the aperture values of the particular pipes are initially spatially uncorrelated lognormally distributed. Different degrees of aperture variability were examined to assess the sensitivity of aperture variability on karst evolution and the resulting cave patterns. Dissolutional growth was studied as the coefficient of variation of the initial aperture data of the single protoconduits varies. In comparing the cumulative frequency distributions of uniform and variable initial aperture fissures, the impact of aperture variability on dissolutional growth was analysed. It was found that a small degree of heterogeneity led to cave patterns similar to those obtained with uniform initial apertures. However, with increasing heterogeneity the karstification process decelerates and a significant amount of variability between the different realisations followed. In an ensemble average sense, the aperture variability is determining the temporal development of the cave patterns and generally decelerates the karstification process, but appears to be of minor relevance regarding the general structure and geometric properties of the cave patterns evolving in the long-term. For a highly permeable formation conduit development generally leads to bimodal aperture distributions independent of the degree of aperture variability. In the case of lowly permeable rock formations an increasing degree of heterogeneity is found to have an impact on the structure of the conduit system during the early stage of karstification. In this case, the cumulative frequency distribution shows to some extent a bimodal structure and there is a high variability between different realisations. In the long-term, however, the differences between the individual realisations disappear and a smooth transition from narrow protoconduits to large-diameter conduits evolves just like in settings with a low initial heterogeneity.

4. Conclusions

The numerical models designed in the present project provide a simplified representation of the hydrogeologic environment found in the karst settings of the Western Ukrainian type. Our results reveal the influence of the spatial extension of the discharge area, the hydraulic conductivity of the rock formation, the variability of initial apertures, and the chemical saturation of the water on cave patterns evolving. Although the various scenarios yield different cave patterns, all of them agree qualitatively well with features of the various cave systems in the Western Ukraine, e.g., the decrease in the number of vertical conduits from bottom to top of the gypsum and the pronounced horizontal passages.

Our model scenarios suggest that the permeability of the entire rock formation is a crucial factor that controls the frequency distribution of conduit diameters in hypogene speleogenesis. Rehrl et al. (2008b) demonstrated that a bimodal distribution can be only obtained if the increase of flow rates is not suppressed due to the low permeability of the rock formation. If permeabilities are sufficiently low the aperture distribution will be characterised by a smooth transition from nearly undeveloped, narrow protoconduits to well-developed large-diameter conduits. Thus the entire network of protoconduits is uniformly widened at a low rate. In part, this also applies to situations where the inflow to the soluble unit is already at a high chemical saturation. The bimodality of the frequency distributions in those scenarios appears to be less pronounced than in the basic setting.

In principle, quantitative analysis of aperture distributions in the field should make it possible to assess whether or not the conduit system developed under a suppressed flow regime. In practice, however, this data can hardly be obtained in deep-seated settings, and if the formations become better accessible due to uplift, the environmental conditions (permeability of aquifers and confining beds, regional hydraulic gradients) may change in a way that favours competitive conduit development such that the former aperture distribution cannot be recognised anymore.

Furthermore, our results suggest that the initial aperture variability controls the temporal development of conduit systems in hypogene settings. With increasing degree of heterogeneity the number of conduits developed after a given time period decreases. In the long-term, however, the differences in the initial heterogeneity appear to be overridden and the conduit systems approach similar patterns. As pointed out by Birk et al. (2003), boundary conditions are likely to change with time, e.g., due to the incision of valleys. In that case, the differences in the temporal development of the conduit system in settings with different initial heterogeneity might have an impact on the cave pattern evolving in the long-term. Thus, we suggest that an improved characterization of aperture widths in karst rocks can be useful for improving our understanding of the speleogenesis and the morphology of cave systems developed in various types of settings.

More generally, our results suggest that numerical modelling is not only useful for studying the general interactions of physical and chemical processes governing karst evolution. The translation of site-related conceptual models to numerical model scenarios can provide insight into speleogenetic mechanisms and controlling factors of karst evolution in specific types of settings. The numerical models presented herein are still highly simplified. Thus future work will have to substantiate the conclusions drawn here using more complex models (e.g., three-dimensional models explicitly representing the observed discordance of fissure networks) based on more detailed field data (e.g., frequency distributions of aperture widths).

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Rehrl, C., Birk, S. & Klimchouk, A. B. (2009, submitted): Influence of initial aperture variability on conduit development in hypogene settings. - Zeit. f. Geomorph.

Appendix: List of Publications and Presentations

Peer-reviewed papers

Rehrl, C., Birk, S., Klimchouk, A. B. (2009): Conduit development in hypogene settings: Development and validation of numerical models by field evidence. Zeitschrift für Geomorphologie, submitted.

Rehrl, C., Birk, S., Klimchouk, A. B. (2009): Simulating the development of solution conduits in hypogene settings. In Conference Proceedings – Hypogene Speleogenesis and Karst Hydrogeology of Artesisan Basins, Chernevitsy, Ukraine, May 12-17, 2009, submitted.

Rehrl, C., Birk, S., Klimchouk, A. B. (2008): Conduit evolution in deep-seated settings: Conceptual and numerical models based on field observations. Water Resources Research **44**, W11425, doi:10.1029/2008WR006905.

Rehrl, C., Birk, S., Klimchouk, A. B (2008): Numerische Modellierung der Karstgenese in mehrschichtigen artesischen Systemen. In: Marschallinger R., Wanker, W. (eds.), Computeranwendungen in Hydrologie, Hydrogeologie und Geologie - Beiträge zur COG-Fachtagung Salzburg 2007. Wichmann, Heidelberg: 71-78.

Abstracts

Hubinger, B., Rehrl, C., Birk, S. (2008): Einfluss der Karstgenese auf Aquiferheterogenität und Transporteigenschaften: Untersuchungen mittels numerischer Modellierung. Journal of Alpine Geology (Mitt. Ges. Geol. Bergbaustud. Österr.) **49**: 47.

Rehrl, C., Birk, S. (2008): Modellierung der Aquifergenese in Karstgebieten. Journal of Alpine Geology (Mitt. Ges. Geol. Bergbaustud. Österr.) **49**: 85.

Reimann, T., Rehrl, C., Geyer, T., Liedl, R., Birk, S., Sauter, M. (2008): Anwendung von Hybridmodellen in Karstgrundwasserleitern. Proc. Tagung Numerische Grundwassermodellierung: Konzeption, komplexe Anwendung, Entscheidungsgrundlage, Graz, June 24-25, 2008: 34-37.

Rehrl, C., Birk, S., Klimchouk, A. B (2008): Site-related numerical models of conduit development in hypogene settings. In: Flow and Transport in Heterogeneous Subsurface Formations: Theory, Modelling and Applications. IAHR International Goundwater Symposium, Istanbul, June 18-20, 2008: 194.

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Talks on Scientific Conferences

Rehrl, C., Birk, S., Klimchouk, A. B. (2009): Simulating the development of solution conduits in hypogene settings. Internat. Conf.: Hypogene Speleogenesis and Karst Hydrogeology of Artesisan Basins, Chernevitsy, Ukraine, May 12-17, 2009. accepted.

Hubinger, B., Rehrl, C., Birk, S.: Einfluss der Karstgenese auf Aquiferheterogenität und Transporteigenschaften: Untersuchungen mittels numerischer Modellierung. Pangeo, Vienna, September 22-25, 2008.

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