

## PROGRAM AND BOOK OF ABSTRACTS

## UNCE Student Conference 27<sup>th</sup> of April 2023

Center for Geosphere Dynamics UNCE/SCI/006 2018/2023

> Faculty of Science, Albertov 6 Charles University, Prague

## Program

	<u>Time</u>	Title	<u>Session</u>
14:00 Opening Remarks			
Alda Vieira	14:15	The fate of legacy mercury in the soils surrounding an abandoned iron and mercury ore mine	Geochemistry and Mineralogy
Petra Venhauerová	14:30	The stability of poorly crystalline arsenate phases under varying levels of phosphate	
Lucie Kunstmüllerová	14:45	Bivalves as palaeoecological markers at the onset of the OAE2 event (Bohemian Cretaceous Basin, Czech Republic)	Palaeontology
Ondřej Kohout	15:00	A possible new species of lower Turonian ammonite from Bohemian Cretaceous Basin and clear evidence of mosasaur – ammonite predation in BCB	
Coffee break 15:15			
Marian Takáč	15:30	UAV Magnetometer Survey over Acraman Crater	Applied Geosciences
Václav Santolík	15:45	Arc evolution on an extended continental crust: Evidence from the Ediacaran Avalonian-Cadomian belt, Teplá-Barrandian unit	
Rodrigo Polo-Mendoza	16:00	Contribution of Deep Neural Networks (DNNs) in the prediction of soil geotechnical parameters	
Maria Pico-Duarte	16:15	Enhancement of a hydro-mechanical hypoplastic model for unsaturated fine-grained soils accounting for small strain stiffness	
16:30 Closing Remarks			

## The fate of legacy mercury in the soils surrounding an abandoned iron and mercury ore mine

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Stable mercury (Hg) isotope ratios, complemented by solid phase Hg speciation data, were determined in two soil profiles that were sampled at different distances from a former mining and smelting site for Fe and Hg ores. The soils were predominantly composed of insoluble cinnabar (HgS). A portion of Hg(II) was weakly bound to mineral soil particles and these more soluble Hg species likely played a key role in soil biogeochemical processes. The Hg isotope data showed slight differences between the primary cinnabar ( $\delta^{202}$ Hg: -0.78 to -1.11‰) and studied soils, and relatively small  $\delta^{202}$ Hg variations within the soil profiles. Close to the mining area, the soil profile had more negative  $\delta^{202}$ Hg values in the organic and organo-mineral layers (-1.25 to -1.15‰) than in the mineral horizons (-0.89 to -0.82‰), where  $\delta^{202}$ Hg values matched its bedrock (-0.89‰) and the HgS signatures. More negative  $\delta^{202}$ Hg signatures in the top horizons suggest the deposition of isotopically lighter Hg. The soil profile sampled down-slope from the mining area showed a more negative shift in  $\delta^{202}$ Hg signatures (-1.44 to -1.03‰), and is similar in organic and mineral horizons. This shift may point to certain soil processes that control the isotopic fractionation, probably Hg(II) adsorption onto mineral particles (e.g., secondary Fe/Mn oxides).

Acknowledgements: This study was partially supported by institutional funding from the Centre for Geosphere Dynamics (UNCE/SCI/006).

# The stability of poorly crystalline arsenate phases under varying levels of phosphate

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While the competition between arsenic and phosphate for sorption sites has been widely studied, the stability of poorly crystalline or amorphous arsenic phases at elevated phosphate levels remains unclear. This study investigated the impact of different aqueous levels of phosphate (0 mM, 0.5 mM, and 50 mM) on the stability of amorphous ferric arsenate (AFA, FeAsO<sub>4</sub>·xH<sub>2</sub>O) and poorly crystalline vukonite (Yuk,  $Ca_2Fe_3(AsO_4)_3(OH)_4 \cdot 4H_2O$ ) in both synthetic phases and natural phases occurring in composite materials (mining waste and soil). The stability of these arsenate mineraloids was examined using a batch experiment and monitored for a year. The findings revealed that the extracted As from all solid samples increased with increasing phosphate concentrations. The total As content in synthetic solids dropped by 50 % at 50 mM phosphate solution compared to 0 mM, while the P levels reached > 80 g/kg. However, no phase transformations were detected by XRD analysis in the synthetic phases. Chemical microanalyses of the synthetic phases indicated that As was substituted in the structure of AFA and Yuk by phosphorus, implying their low stability at high phosphate levels. In addition, substantial release of As (~13 %) and sequestration of P (up to 6.5 g/kg) was observed in the AFA-rich waste and Yuk-rich soil, but no chemical changes were documented in the AFA and Yuk phases. Microprobe analyses suggested that the major mechanism of As and P exchange in the mine waste and soil involved sorption processes with the omnipresent Fe (oxyhydr)oxides. These findings suggest that effective As sorbents such as Fe (oxyhydr)oxides could effectively suppress the instability of amorphous or poorly crystalline arsenate phases at high phosphate conditions.

Acknowledgments: This research was supported by the Grant Agency of Charles University (GAUK no. 790120), Czech Science Foundation (GAČR no. 22-27939S), and Center for Geosphere Dynamics (UNCE/SCI/006).

### Bivalves as palaeoecological markers at the onset of the OAE2 event (Bohemian Cretaceous Basin, Czech Republic)

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The Ocean Anoxic Event (OAE2) at the Cenomanian-Turonian boundary presents a unique record of gradual global warming and its effects on benthic organisms. In this study, we present a statistical evaluation of bivalve assemblages from the onset of the event from the Pecínov member in the Bohemian Cretaceous Basin (BCB). While this locality's other molluscan fauna (ammonites, inoceramids) has been extensively studied, the bivalve association and its potential for paleoenvironmental reconstructions have received little attention.

Fossil bivalve assemblages are generally recognised as reliable palaeoecological indicators of the sea bottom environment due to their abundance in the fossil record, para-autochthonous preservation and the valuable information that can be gleaned from their presence. As primarily filter feeders, bivalves play a significant role in ecosystem dynamics and are highly sensitive to environmental changes. Therefore, variations in bivalve species composition, diversity, and abundance can provide essential clues about past environmental conditions such as temperature, salinity, nutrient availability, and substrate type. Additionally, the functional morphology of bivalves can reveal specific adaptations to environmental conditions, providing further insight into the ecological context in which they lived.

The assemblage from the locality is divided into guilds based on their ecospace utilisation using statistical and population analysis resulting in a new palaeoecological interpretation. Close attention was also dedicated to the preservation, fragmentation, orientation of shells, their spacing, and their position to each other. The assemblage is strongly dominated by infaunal suspension feeders, followed by semi-infaunal suspension feeders. The near absence of free-living epifaunal bivalves was probably caused by the very fine, muddy substrate and water turbidity, a significant limiting factor for many epifaunal species, especially in shallow, near-shore conditions. The infaunal deposit feeders are also present but comparatively rare, indicating a nutrient-rich environment with a sufficiently high energy level to keep organic matter in suspention. The *Cucullaea glabra - Pseudoptera anomala* assemblage is considered to be deposited during normal, shallow marine conditions.

Acknowledgements: This research was supported by the Czech Science Foundation (GAČR no. 21-30418J), and the Center for Geosphere Dynamics (UNCE/SCI/006).

### A possible new species of lower Turonian ammonite from Bohemian Cretaceous Basin and clear evidence of mosasaur – ammonite predation in BCB

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We present preliminary results from an ongoing study of a new (sub)species of ammonite collected from the lower Turonian sediments of Ždánice in the vicinity of Kouřimi in the Bohemian Cretaceous Basin. The collection consists of 38 specimens preserved as inner moulds. The ammonites represent a range of morphological features that are distinct from other known ammonite species from the same formation. These include mainly unique ornamentation which will be discussed with great emphasis. The preliminary analysis suggests that this collection represents a new species of ammonite, which has yet to be formally described. This new species adds to the growing diversity of ammonites from the Bohemian Cretaceous Basin, and provides valuable insights into the evolutionary history and biogeography of these extinct cephalopods. Further studies, including morphometric analysis and comparisons with other ammonite taxa, will be necessary to fully understand the significance of this new species and its relationships to other members of the ammonite fauna.

In addition to the new species of ammonite, another ammonite will be briefly present - a single specimen of *Mammites nodosoides*, which displays a clearly preserved shell with a distinctive pattern of bite marks, likely caused by the teeth of mosasaur predator. The presence of such predation marks provides valuable information on the ecological interactions between these organisms and sheds light on the paleoecology of the lower Turonian of the Bohemian Cretaceous Basin.



Fig. 1: Schematic view of mosasaur bite marks on the shell of Mammites nodosoides

**Acknowledgements**: I would like to express my gratitude to Professor Martin Košťák and Dr. Martin Mazuch my, for their invaluable support and guidance throughout this research. I am also thankful to Dr. Jan Sklenář and the Palaeontologic department of the Czech National Museum for their assistance and resources. This research project was made possible in part by the financial support of UNCE/SCI/006.

### **UAV Magnetometer Survey over Acraman Crater**

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Acraman crater is an impact structure (eroded crater) located in South Australia, north of the Minippa. It is the remnant of a crater that formed after the impact of an extraterrestrial body approximately 580 million years ago (Williams and Gostin, 2010). At the center of the impact structure is Lake Acraman, round shaped lake with a diameter of approximately 20 km. The lake is relatively shallow and usually dried out. The current magnetic map of the Acraman area is based on aeromagnetic surveys done as part of the Geological Survey of South Australia program. From airmag surveys, a local magnetic anomaly is evident. A significant magnetic anomaly is located over the central part of the crater (where the salt basin of Lake Acraman is). Local magnetic anomalies represent variations in the magnetic field and are often caused by changes in geology. Magnetic signature in the Lake Acraman area was discussed by (Williams et al., 1996) where the central anomaly appeared to be dipolar. We performed the most detailed UAV magnetometer survey in the area of the primary magnetic anomaly. We used a drone for the measurements, which allowed us to perform measurements lower above the ground level and in a lower profile spacing than is possible with a conventional aeromagnetic survey. Thanks to the high density of the data, it is possible to visualize the central magnetic anomaly in the best resolution to date. Our data show the most detailed view of the main magnetic anomaly and refine its shape. The new data have the potential to reveal the cause of the central anomaly, whether it is formed by natural geology, or possibly by the uplift of the lower layers of rocks due to the impact, or whether there could be some residue of an impact body below the surface.

Fig. 1: Flight path of the UAV with measured data preview.



Williams, G.E., Gostin, V., 2010. Geomorphology of the Acraman impact structure, Gawler Ranges, South Australia. Cad. Lab. Xeoloxico Laxe.

Williams, G.E., Schmidt, P., Boyd, D.M., 1996. Magnetic signature and morphology of the Acraman impact structure, South Australia. AGSO J. Aust. Geol. Geophys. 16, 431–442.

# Arc evolution on an extended continental crust: Evidence from the Ediacaran Avalonian-Cadomian belt, Teplá-Barrandian unit.

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During the Ediacaran period, an extensive accretionary orogen developed on the northern margin of the supercontinent Pannotia: the Avalonian-Cadomian orogen. Remnants of this orogeny are preserved in the form of isolated terranes incorporated in the Late Palaeozoic Variscan collisional orogen and are dispersed throughout North America, Northern Africa, Europe and Eastern Asia. Despite the vast amount of data collected over the decades of research, the overall nature of the Avalonian-Cadomian orogen, the timing of geotectonic events, as well as the position of individual terranes within the Orogen is still a matter of debate.

The aim of our study is to describe the evolution of the Davle volcanic complex (DVC), one of the best-preserved arcs in the Cadomian part of the Orogen, situated in the Teplá-Barrandian unit of the Bohemian Massif. Using detailed field observations, petrography, major- and trace-element concentrations, Nd-Hf isotopic values as well as LA-ICP-MS U-Pb zircon dating, we were able to introduce a complex evolutionary picture of the arc, divided into three stages. The first stage comprises a volcano-plutonic association of andesite, dacite, rhyolite and orthogneiss. The U-Pb zircon data from the orthogneiss dates this stage to 600 - 590 Ma. The whole suite is characterized by low TiO<sub>2</sub> contents (0.2–0.5 wt.%), enrichment in light-ion-lithophile-elements (LILE), intermediate ENd values (+3.6 to -5.1), and may be internally connected by assimilation-fractional crystallization (AFC) process, which is demonstrated by geochemical modeling. The second stage reflects the termination of the volcanic activity and development of post-arc basin covering the former arc. The laminated tuff layers at the base of the second stage exhibit different geochemical features compared to the volcanic rocks from the first stage including an increase in  $TiO_2$  (0.2 – 0.7 wt.%) demonstrating a change in magmatic source. The geochemical features of the overlying sedimentary rocks (Lečice Member and Štěchovice Group) gradually shift towards derivation from more evolved continental crust as documented by increase in lithophile-element contents like Nb (from 3 to 14 ppm). Th (from 2 to 9 ppm), and Zr (from 50 to 200 ppm), but decrease in  $\epsilon$ Nd values (from +0.4 to -7.1). The third stage, comprising an intrusion of subvolcanic trondhiemite and related rhyolite dykes, demonstrates an intra-arc extension. The highly positive ENd values (+4.8 to +8.4) and intra-oceanic-like geochemical features point to juvenile magmatic sources with minimal crustal contamination. The three-stage evolution of the DVC is interpreted as representing a termination of the volcanic arc activity on an extended continental crust: from a fringing arc in the first stage to an intra-arc extension in the last stage.

# Contribution of Deep Neural Networks (DNNs) in the prediction of soil geotechnical parameters

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Determining the Soil Geotechnical Parameters (SGP) is essential for designing a wide range of engineering infrastructures, such as backfills, buried high-voltage cables, embankments, footings, nuclear waste disposal facilities, pavement structures, piles, and retaining walls. Notably, the experimental determination of these parameters is time-consuming and typically requires the operation of sophisticated laboratory devices. Unfortunately, in many cases, there are insufficient resources (in terms of time and budget) to carry out these tests. Therefore, to overcome these limitations, it is common in engineering practice to utilize indirect estimation methods. However, the main problem with applying these techniques to forecast the SGP is that the soils are highly variable, so traditional mathematical procedures usually present significant predictive errors.

In recent years, soft-computing approaches are gaining elevated notoriety to overcome the limitations of conventional mathematical expressions. In this way, it has been possible to develop computational models with predictive capabilities more prominent than the typical ones exhibited by correlation-like expressions. Nevertheless, these computational models have not been widely employed in geotechnical engineering to forecast SGPs. In the light of the above, in this research, two Deep Neural Network (DNN) models are proposed to estimate some SGPs, namely maximum dry unit weight ( $\gamma_{d(max)}$ ), optimum moisture content ( $w_{opt}$ ), California Bearing Ratio (CBR), and Resilient Modulus (M<sub>r</sub>).

In this first DNN model, the objective was to forecast the  $\gamma_{d(max)}$ ,  $w_{opt}$ , and CBR. For this purpose, the grain size diameters  $(D_{10}, D_{30}, D_{50}$  and  $D_{60})$ , the coefficients of uniformity  $(C_u)$ , and the coefficients of curvature  $(C_c)$  were considered as input variables. Meanwhile, the second DNN model intends to estimate the M<sub>r</sub> utilizing as input variables the grain size distribution (percentage of soil that passes through the following sieves: 3 in, 2 in, 1.5 in, 1 in, 0.75 in, 0.5 in, 0.375 in, No.4, No .10, No.40, No.80, and No.200) and the stress conditions (i.e., bulk stress and octahedral shear stress). For both computational models, performance assessments were conducted, taking as benchmarks some conventional mathematical formulas. In all cases, it was possible to demonstrate that the proposal based on machine learning yielded results with more remarkable accuracy and precision. Thus, the main contribution of this research to the state-of-the-art is the development of DNN models capable of estimating some of the most critical SGPs (for engineering applications) with high accuracy by merely using the granulometry of soils.

Acknowledgements: The authors appreciate the financial support given by the grant No. 21-35764J of the Czech Science Foundation. Likewise, the authors acknowledge the institutional support of the Center for Geosphere Dynamics (UNCE/SCI/006).

### Enhancement of a hydro-mechanical hypoplastic model for unsaturated fine-grained soils accounting for small strain stiffness

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The increase in larger extreme seasonal and daily moisture variations caused by global climate change can influence the behavior of geotechnical structures by inducing coupled hydro-mechanical loads. For this reason, from a numerical point of view, robust constitutive models that are able to predict the couple-hydro-mechanical behavior of fine-grained soils, combined with predictions of history-dependent stiffness evolution at small strains are needed. The present work presents the enhancement of a hypoplastic model for unsaturated fine-grained soils. For this purpose, a smoothed hysteretic Water Retention Curve was incorporated into the model formulation to obtain more realistic predictions of the non-linear dependency of degree of saturation and suction. Afterwards, the constitutive model was calibrated using experimental data available in the literature of a completely decomposed tuff from Hong Kong. The capabilities of the extended model for predicting the cyclic behavior of unsaturated soils were also studied by simulating cyclic constant water triaxial tests at different suctions. The results showed that the extended model is able to predict with more accuracy the cyclic hydro-mechanical behavior of the decomposed tuff when suction-dependency is added to one of its small strain stiffness parameters.



*Fig. 1:* Water retention behavior curve at Experimental data by Ng et al. (2009) (Measured) against model predictions (Computed).

C.W.W. Ng, J. Xu & S.Y. Yung (2009). Effects of wetting-drying and stress ratio on anisotropic stiffness of an unsaturated soil at very small strains. Canadian Geotechnical Journal , 46, 9, 1062-1076.

Acknowledgements: The authors appreciate the financial support given by the grant No. 21-35764J of the Czech Science Foundation and the Center for Geosphere Dynamics (UNCE/SCI/006). The first author acknowledges the financial support given by the Charles University Grant Agency (GAUK) with project number 260422.