2. Description of individual research project and research results achieved to date:

**Motivation**
An on-going challenge for environmental monitoring is the interpretation of temporal and spatial trends from monitoring data (Richards et al. 2012). Mostly, this data and the relation in between are complex, multivariate and nonlinear. In particular, there are only few studies dealing with the roadside soil topic of soil solution concentrations related to the run-off concentrations of high ways (i.e. Dierkes and Geiger 1999; Kocher et al. 2005; Hjortenkrans et al. 2008; Kluge and Wessolek 2011; Kluge et al. 2014; Kluge et al. 2016; Werkenthin et al. 2016). In some scientific papers, relations between trace elements and boundary conditions such as pH, soil solution EC and climatic factors are mentioned for interpreting transport and leaching, but the temporal and spatial variations were not yet in the scientific focus, because such complex and long-term data is rare and not easily available.

Due to the soil profile heterogeneity, some experimenters found that it is more desirable to use stochastic models rather than constant values in predicting the future concentration of soil solutes and soil moisture. For this, the parameters of stochastic transport models are treated as random variables with discrete values assigned according to a given probability distribution (Zhang et al. 2009; Fortin et al. 2010, Park et al. 2005; Green et al. 2007; Khazaei et al. 2008; Aljoumani et al. 2012; Aljoumani et al. 2015; Aljoumani et al. 2017).

Within this context this project is planned to achieve three objectives:

- Understanding and predicting temporal trends and patterns of trace elements of the soil solution of roadside soils, taking into account: rainfall intensities, humidity, evapotranspiration, infiltration, soil moisture, runoff concentrations and volumes, soil solution concentrations in different depths, soil temperatures, soil solution EC ($\sigma_p$), pH, and data from a climate station.
- Estimating the pore water EC ($\sigma_p$) from TDR/FDR probes. To get $\sigma_p$ from the TDR/FDR probes, we need to convert the bulk electrical conductivity ($\sigma_b$) that will be measured by probes from the lysimeter to $\sigma_p$ by evaluating the linear relationship between soil dielectric constant ($\varepsilon_b$) and $\sigma_b$ under urban soil conditions.
- Evaluating the linear changes of soil temperature ($\Delta t$) - logarithm of time (lnT) model using single heat probe to estimate precisely soil thermal conductivity in laboratory conditions taking into account the effect of salt on the soil thermal conductivity and predicting the soil temperature at deeper depths by measuring upper depths in lysimeter conditions.

**Methods**
The above-mentioned objectives are based on the following hypothesis:

- To evaluate temporal trends and variations of metal concentrations in the soil solution of roadside soils, we test the hypothesis that metals concentration follow linear and non-linear relationships based on the following data: rainfall intensities and volumes, runoff concentrations and volumes, soil depth, soil temperature, soil solution EC ($\sigma_p$), pH, hydraulic conductivity, and climate data. Dissolved metals sampled from Highway lysimeter (Fig 1).
- To estimate precisely the $\sigma_p$ by TDR/FDR data obtained from urban soils, this study will test the hypothesis that there is a stochastic component in the linear relationship between $\sigma_b$ and $\sigma_b$.
- To estimate the thermal conductivity by single heat probe using the De Vries model, we test the hypothesis that there is a stochastic component in the linear relationship between $\Delta t$ and lnT.
- To predict the time series of soil temperature and solute transport, we test the hypothesis that the observations are correlated to each another (soil temperature data collected from lysimeter – T1 project, Fig3).
The following working steps need to be done for proving the hypothesis:

(i) Using the Generalized Additive Mixed Models (GAMM) to analyze the above mentioned field data from lysimeter, lab and climate.

(ii) Using of a Dynamic Linear Model (DLM and a Kalman Filter to convert $\sigma_b$ to $\sigma_p$ by studying the linear relationship between soil dielectric constant ($\varepsilon_b$) and $\sigma_b$ to data obtained from urban soil conditions, then programing these stochastic models and inserting them into Hydrus1D - which is widely used for simulating water flow and solute transport in variably saturated soils and groundwater (Šimůnek et al. 2008). Moreover, the study will use also DLM and Kalman Filter to estimate soil thermal conductivity by evaluating the linear changes of temperature - logarithm of time model.

(iii) Using of Time Series Analysis, Outlier detection and Transferring Function Model to predict the soil temperature and soil solution EC at deeper depths by measuring upper depths.

Current State of Work

For the first work step of this project, monthly data of dissolved Cd, Ni, Cr, Pb, Cu and Zn concentrations in three different roadside soils were measured during a two years lysimeter field study at different depths. The study was used to assess the temporal variation of trace elements and how they were affected by environmental factors. For data interpretation, both analyses of variance (ANOVA) and Generalized Additive Mixed Models (GAMMs) were used. Though ANOVA does not allow estimating clear trends because of using repeated measurements, GAMMs was used to explore the complex behavior of metals in heterogeneous soils by detecting linear and nonlinear trends of metal concentrations in the soil solution.

The modeling approach showed that Cd, Ni, Cr, Pb, Cu and Zn concentrations are functions of different environmental variables, which have either a linear or a nonlinear behaviour (some results in Fig 4). All investigated metals show a common effect by time, pH and depth. Ni and Cr are functions of almost the same
environmental factors used in this study. Moreover, the GAMM model showed the importance to account for the nonlinear temporal variation in metal concentrations. In our study, we explore the nonlinear relationship between Pb, Zn, Ni, Cd concentrations and pH, Cu and EC, Cr and infiltration, Cr, Ni and runoff concentration and between Zn and precipitation, evapotranspiration, soil moisture and surface runoff. The work of this objective resulted in a journal paper which is currently under review (Aljoumani et al. 2018a).

Part of the 2nd work step is achieved (Aljoumani et al 2018b) where a time-varying dynamic linear model (DLM) and Kaman filter (Kf) is used to estimate pore water electrical conductivity (σp). Time series of soil dielectric constant (εb) and bulk electrical conductivity (σb) were measured with Time domain reflectometry (TDR) at different depths in a soil column to modify the deterministic Hilhorst (2000) model into a stochastic model and evaluate the linear relationship between εb and σb in order to estimate precisely σp. As a result, the observed and modeled data of εb match reasonably well (Fig 5).

Figure 4: Explanatory variables of GAMMs, linear and nonlinear effects on the metal concentrations at the investigated roadside soils

Figure 5: Observed and predicted soil dielectric constant at 21 cm depth.
**Future Work Planned**
More laboratory experiments are planned to apply numerical model to estimate pore water EC (2nd work step). The third work step will use data from T1 (1st UWI cohort) to valuate the temporal trend of evapotranspiration and prediction of soil temperature on lysimeter conditions, as well as a laboratory experiment will be applied to estimate the effect of solutes on the soil thermal conductivity.

**Collaboration**
The research is closely linked with project T1 and N2 from the 1st UWI cohort and W2 from the 2nd UWI cohort. By working on the lysimeter soil temperature data obtained from project T1 (1st cohort), we will develop a model to predict the soil temperature at deeper depths by measuring the temperature at lower depths using Time Series Analysis and Transfer Function techniques. This contribution will be strongly linked to the project N2 (1st cohort). Moreover, this project collaborates strongly also with W2 (2nd UWI cohort) by evaluating the temporal trend of precipitation data.

**References**


3. **Description of individual RTG-specific tasks**
   Courses in time series analysis by R to the PhD students of RTG

4. **Statement on career development measures**
After completing my 2 years with UWI, I will achieve a significant improvement in my career as following: First, monitoring water flow and solute transport by using numerical models. In my previous studies I used stochastic model to study them, this project will give me the opportunity to stretch my knowledge in physical and chemical urban soil properties to apply numerical models. Second, getting the opportunity to have experience in teaching during the UWI core course (6 December 2018) and another planned individual course in time series analysis with R to model hydrological data. Third, publishing and doing conferences in new topics to my experience related to urban soils. Moreover, according to the UWI project program and its events, I will meet multidisciplinary group which give me the opportunity to collaborate with them and expand my network. Finally, I would mention to the experience that I learn from the UWI speaker Prof. Hinkelmann in the topic related to the rules for developing a successful research proposal.

<table>
<thead>
<tr>
<th>Participation in or organisation of RTG-related events:</th>
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<tbody>
<tr>
<td>• Summer School (05. – 06.09.2016)</td>
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<td>• Kollegiate Seminar (22.09.2016)</td>
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<tr>
<th>Participation in conferences, congresses, etc., at home and abroad:</th>
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<tr>
<td>2016:</td>
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<td>- EGU General Assembly, EGU2016 (17. – 22.04.2016)</td>
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<td>2017:</td>
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<td>2018:</td>
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5. Individual publications:

I. Articles


II. Conference, poster presentations etc.: