An implementation of environmental databases for physical modeling of water balance and land degradation

Tomasz Stuczyński, Artur Łopatka, Bernadetta Zawadzka, Grzegorz Siebielec

Department of Soil Science Erosion and Land Conservation Institute of Soil Science and Plant Cultivation – National Research Institute ul. Czartoryskich 8, 24-100 Puławy, Poland

Abstract. There is an increasing demand for the rapid and quantitative assessment of different aspects of environmental quality. This is associated with the need for a more efficient and sustainable use of existing resources. It is well established that water deficit is a limiting factor of various soil functions in Poland as sixty percent of soil cover represents a coarse texture of poor water holding capacity. Increasing water retention within the landscape becomes one of the objectives for land management and related policy. This requires a spatial assessment of water retention characteristics and of the soil cover. In post-industrial areas in addition water deficiency impacts on crops and ecosystem can be enhanced by land degradation and contamination. Identification of these processes requires either traditional measurement or application of modeling tools as an alternative. The benefit of modeling is reduction of cost, however these methods can introduce a larger uncertainty to the assessment comparing to traditional surveys. This paper addresses our preliminary results of alternative techniques for modeling of water balance in soils as well as identification of potentially contaminated areas through remote sensing. Topics presented here belong to set of tools our group has been developing in recent years showing a potential of digital data bases and satellite images for identification of major threats to soil functions such as water deficit and contamination. These two land quality assessment methodologies are discussed in this paper to demonstrate alternatives for a better management and protection of environmental resources.

key words: environmental databases, modeling, water balance, soil contamination

INTRODUCTION

An assessment of spatial and multitemporal dynamics of a soil water can be achieved through modeling utilizing soil maps and soil profile data, digital terrain models, and

Corresponding author:

Tomasz Stuczyński

e-mail: ts@iung.pulawy.pl

tel. +48 (81) 8863421 ext. 311, fax +48 (81) 8864547

Received 2 September 2009

weather data. Soil suitability maps developed in Poland with the full coverage for the country, in scale of 1:25000, contain characterization of texture of the soil profile. Utilizing these soil data resources by adapting existing models is difficult as these models usually require a specific soil input according to different texture or soil classification rules. Redefining mapping units to meet the required set of criteria usually involves a significant generalization as there are often no robust transfer algorithms available. In order to fully benefit from a high resolution information derived from digital soil maps we developed a physical spatial model simulating water movement through the soil profile within a river basin.

Dealing with contaminated sites and hot spots is another emerging issue which requires urgent solution to protect water and soil quality in post-industrial areas. These sites and hot spots represent a very small portion of land in Poland which is less than three percent of the total territory, however locally they can contribute to a significant environmental health and food chain risk (Terelak et al., 1997). New environmental law adopted in Poland requires that local authorities at the NUTS-4 level identify and upgrade information on contaminated sites to develop respective reclamation programs. To reduce the cost of detailed studies involving traditional monitoring methodologies we tested the utility of multi-spectral ASTER images to characterize spatial variability of metal concentrations in contaminated land covered with smelter waste deposits in Silesia, post-industrial region of Poland.

There is a number of commercially available models like FEFLOW (Diersch, 2009) or MODFLOW (Harbaugh, McDonald, 1996) on the market with well functioning water balance module. However most of these models are based on an empirical approach and usually require a vast amount of data which is not readily available. On the other hand the existing high resolution data such as soil maps can not be loaded into existing models without conversion which is usually resulting in generalization, loss of specific information and decreasing the robustness of predictions. The objective of our modeling work is to develop a GIS based model calculating water balance within a river basin scale. The prototype of our model being currently developed is thought to retrieve complex physical processes controlling water flow through the soil and the landscape within given river basin boundaries.

The main functions of the model is to predict runoff, moisture and soil matrix potential for any grid cell and time point. Results will be visualized as maps of areas vulnerable to drought and maps characterizing potential for water retention by the soil cover under specific land use. Such a tool can be used to support decision making in water management, for restructuring the land use and to identify best location for restoration of wetlands and ponds to enhance water retention within the landscape.

METHODOLOGY BACKGROUND FOR WATER MODELING

The physical basis for the water balance is given by the continuity equation. The mathematical formula describing this rule is as follows:

$$\frac{\partial \theta}{\partial t} = r - e + \vec{\nabla} \cdot \vec{q}$$

where: θ is the volumetric moisture, r is an intensity of rainfall (the amount of precipitation per time unit, per soil volume unit), e is the intensity of evapo-transpiration as calculated from Penman's equation, and q is water flow.

In the case when the system is open and there is an outlet from the catchments of interest discharging water to a larger basin it is necessary to modify the continuity equation to account for this discharge by using a proper differential formula (Soczyńska, 1989).

The flow in a porous system such as soil is commonly described by Darcy's equation

$$\vec{q} = K(\theta) \vec{\nabla} \left(z + \frac{p(\theta)}{\rho g} \right)$$

where z is the height (depth in the profile), g is gravitational acceleration, ρ is density of water and the resulting differential equation known as Richard's formula describes both water infiltration, sub-surface water movement and capillary movement. There are two functions within Darcy's equation which are dependent on moisture. The conductivity component K(θ) can be derived based on known water retention curves and conductivity coefficient at full saturation. Van Genuchten's equations are commonly used for this purpose. Conductivity in a saturated phase and respective retention curves p(θ) can be assigned to existing textural groups based on data reported in the literature, however it may generate major errors. Therefore we used pedotransfer functions which are enabling prediction of the conductivity and retention coefficients based on parameters such as particle size distribution as tested by Niedźwiecki (2002) for large number of samples representative for the soil cover in Poland.

The water runoff down the slope for a regular (nonstormy) rainfall representing laminar flow can be described by Darcy-Weisbach equation,

$$\vec{q} = \frac{8g}{n\eta} h^3 \vec{\nabla} \left(z + h \right)$$

where η is a viscosity of water and h is a thickness of the water film – the respective differential equation allows to describe both runoff and surface retention. The roughness coefficient n is dependent on soil cover physical characteristic as well as on the type and density of vegetation. The n parameter can be derived from the Leaf Area Index (LAI) which can be generated based on multi-spectral satellite images.

Due to formal similarity between the two above equations describing the flow of water they can be solved in an identical way by ADE (Alternating Direction Explicit) finite differences method (Saulyev, 1964) which eliminates technical problems associated with describing the behavior of water within the contact zone between soil surface and water film.

Since analytical solving of the Richards non-linear differential parabolic equation is impossible other computing methods need to be applied. One of the most popular approach is using the method of finite differences. The principle applied here is replacing simple derivatives with respective differential quotients. The right side of the differential formula is given as F.

$$\begin{aligned} \frac{\partial \theta}{\partial t} &= F(\theta(t)) \\ \frac{\partial \theta}{\partial t} &= \lim_{\Delta t \to 0} \frac{\theta(t + \Delta t) - \theta(t)}{\Delta t} \\ & \downarrow \\ \theta(t + \Delta t) &\approx \theta(t) + \Delta t F(\theta(t)) \\ \theta(t + 2\Delta t) &\approx \theta(t + \Delta t) + \Delta t F(\theta(t + \Delta t)) \\ \theta(t + 3\Delta t) &\approx \theta(t + 2\Delta t) + \Delta t F(\theta(t + 2\Delta t)) \\ \vdots \end{aligned}$$

From a definition of the derivative it is evident that the differential quotient provides a better assessment of the derivative as the Δt gets smaller. Therefore moisture after time Δt from a given t can be written as a function of moisture and F at the given t. Replacing time t by time t + Δt in the first equation produces a second formula allowing to calculate soil moisture after time $2 \Delta t$ from the t time point. This procedure can be continued until the required time of a simulation is met.

Spatial derivatives placed on the right side of differential equation can be dealt with in a similar way. The time was divided into time ranges of the length of Δt and the space is divided into rectangular blocks of a dimension Δx , Δy and Δz . With the increasing resolution of time and space the derivatives are calculated with an increasing accuracy and the terrain characteristic is more accurately depicted.

Increasing the accuracy of simulations is achieved by shortening the time range Δt and by decreasing grid size, however it significantly extends the time needed for computing.

The external input to the model include rasterized soil data, watershed boundaries, DEM (Digital Elevation Model) and weather daily data. The simulation process starts from assuming a probable distribution of water in a soil profile and continues assuming steady averaged rainfall until an equilibrium is reached. Knowing the ground water level is helpful for this equilibration process. The distribution of water at the equilibrium stage is a starting point for further computing. The final results given as distribution of moisture or matrix potential are stored in a spatial database which allows further GIS analysis and visualization.

SOIL MOISTURE MODELING RESULTS

Visual basic was used to develop the computing tool which was based on the above modeling principles. The spatial and temporal resolution can be defined by the user, however this strongly depends on the size of modeled catchment since computing capacity of PCs is still a limiting factor. Practically, for catchments larger than 10000 km² 100×100 m grid is recommended, whereas smaller units can be modeled using 30×30 m grid. Further increase of the spatial resolution is limited by the grid size of the available digital elevation model.

Preliminary validation was run by using lysimiter data for one vegetation season and is demonstrated for a loess soil profile at depth of 30, 54 and 86 cm (Figure 1). The calibration is mainly focused on adjusting values of coefficients accounting for evapo-transpiration. As shown on



Figure 1. Measured (dots) and simulated (line) soil moisture.

graphs the measured and predicted moisture are in a good agreement for the upper layers ($R^2 = 57$) whereas with depth the accuracy of the prediction decreases ($R^2 = 30$ and $R^2 = 16$). In order to improve the quality of predictions it is necessary to consider number of different concomitant processes which have an impact on the water flow within the landscape. One of the main difficulties comes from the behavior of air in soil pores after intense rainfall events – increasing the pressure caused by the movement of water significantly slows the infiltration (Wangemann et al., 2000).

Another important aspect to consider is the interception of water by the vegetative cover (Muzylo et al., 2009) – water retained on plant surfaces flows to the soil surface with a delay and is partially evaporated, which affects the actual amount of water reaching soil.

It is known that the direction and magnitude of the runoff are strongly affected by changes in soil physical properties controlled by soil management, land use type and tillage practices, however at this point the available data does not allow using it for modeling purposes at larger scale.

The obtained results encourage us to test the model within a pilot catchment.

Presented methodology holds significant potential for spatial assessment of crops under water stress, however it requires further adjustment and calibration.

USE OF REMOTE SENSING FOR IDENTIFICATION OF METAL CONTAMINATION IN SMELTER WASTE DEPOSITS IN SILESIA

Spatial identification, risk assessment and reclamation of contaminated sites becomes a serious challenge in many post industrial regions. For example smelter and mining waste deposits are scattered throughout Silesia and contribute to degradation of terrestrial ecosystems. Heavy metals present in these deposits are mobilized through wind erosion, runoff and leaching to ground and surface waters.

One of the aims of the EU Soil Thematic Strategy, being currently developed, is to create framework for identifying monitoring and managing risk associated with historical contamination. Traditional approaches to soil characterization involving sampling in the field and laboratory analysis are laborious and expensive. Frequently, precise delineation of a hot spot requires collection of a large number of samples in order to detect spatial dependence and enable interpolation which would meet basic rules of geo-statistics. Alternatively, remote sensing utilizing multi-spectral images seems to provide a good potential for detection of disturbed and waste land. Interpretation and classification of satellite images have been extensively used to distinguish between different land use types including degraded areas such as waste landfills and physically disturbed land surfaces. Hyper-spectral air photographs were used in a pilot JRC's project to detect metal contaminated sites in

a number of European countries (Bidoglio, personal communication). Reflectance spectroscopy was used to characterize contamination, resulting from metal tailings spill in Spain after the accident in Aznalcollar, Spain (Kemper and Sommer, 2002).

Within last few years there were new sources of satellite data introduced such as 14m ASTER images. The Advanced Spaceborne Thermal Emission and Reflection Radiometer (ASTER) is an advanced multi-spectral imager that was launched on board NASA's Terra spacecraft in December, 1999. ASTER covers a wide spectral region with 14 bands from the visible to the thermal infrared with high spatial, spectral and radiometric resolution. The amount of spectral information offered by ASTER seemed to hold good promises to find a quantitative relationship between metal content and reflectance in some spectral bands. To test this hypothesis zinc and lead smelter waste deposits located in Silesia were sampled to measure total concentrations of Zn Pb and Cd using classical analytical methods.

ASSESSMENT METHODOLOGY

Sampling area included 7 zinc and lead waste piles located in different sites throughout Silesia. These sites were known for tremendous spatial variability of metals' content and their mobility. Spectrally similar clusters were identified on ASTER image to design sampling protocol. Composite samples were taken within these clusters by collecting 15 individual subsamples within a radius of 30 m from georeferenced central point of each cluster. Identification of these pre-selected sampling points were achieved through GPS navigation with an accuracy of 1 m. Individual subsamples were merged and mixed to form a homogenous composite sample representative for the surveyed area. Samples were brought to the laboratory, air-dried passed through 8 mm sieve, ground in an agate mortar, and digested in *aqua regia*. Zn, Pb, Cd and other metals were measured using atomic absorption spectroscopy.

Spectral data were averaged for the nine pixels surrounding the central pixel identified by georeferenced sampling point. Correlation was used to characterize relationships between reflectance and metal content in the waste surfaces.

RELATIONSHIP BETWEEN REFLECTANCE AND WASTE PROPERTIES

Data shown in Table 1 indicate that there is a strong relationship between reflectance in short infrared bands (4–9) and number of chemical indicators measured for surfaces which were not covered by vegetation due to metal toxicity. Correlation coefficients in this region are usually above 0.80 which enables to explain over 60 percent of variability of such properties as organic matter (OM), Zn, Ni and Mn. Figure 2 shows an example for Zn. Visible band No. 1 is strongly correlated with Na and Cu content. Thermal bands (10-14) do not seem to be useful indicators of waste surface properties. For surfaces covered with vegetation there were also significant correlations between reflectance and metal concentrations, however respective coefficients were much lower than for barren surfaces (Table 2). Moreover, for vegetated areas the most significant correlations were found for near-infrared wavelength (band 3) as opposed to barren sites for which short infrared bands were much better indicators of metal content. Significant correlation was also observed in thermal region for OM, Zn, Pb and Cd in

Table 1. Correlation coefficients between reflectance in 14 ASTER bands and selected chemical properties of smelter waste deposits barren of vegetation*.

Band No.	Spectral range [µm]	ОМ	Cd	Zn	Pb	Cu	Ni	Cr	Fe	Ca	K	Na	Mn
1	0.52-0.60	0.23	0.09	-0.10	-0.57	-0.87	-0.36	-0.30	-0.41	0.17	-0.65	-0.91	0.47
2	0.63-0.69	-0.24	0.05	-0.06	-0.17	-0.54	-0.31	-0.41	-0.27	0.54	-0.59	-0.53	0.46
3	0.78-0.86	-0.01	0.49	0.51	0.02	-0.34	0.27	0.40	0.05	0.12	-0.45	-0.59	0.58
4	1.60-1.70	-0.56	0.66	0.80	0.43	0.01	0.56	0.44	0.41	0.56	-0.56	-0.27	0.83
5	2.145-2.185	-0.94	0.71	0.87	0.72	0.48	0.80	0.28	0.71	0.80	-0.43	0.31	0.75
6	2.185-2.225	-0.80	0.71	0.89	0.65	0.32	0.74	0.43	0.62	0.70	-0.46	0.08	0.80
7	2.235-2.285	-0.81	0.56	0.78	0.60	0.41	0.72	0.43	0.70	0.66	-0.35	0.21	0.71
8	2.295-2.365	-0.83	0.68	0.83	0.57	0.45	0.82	0.29	0.76	0.74	-0.41	0.30	0.75
9	2.360-2.430	-0.92	0.66	0.74	0.58	0.48	0.76	0.04	0.72	0.84	-0.44	0.41	0.70
10	8.125-8.475	0.24	0.25	-0.11	-0.66	-0.55	-0.08	-0.70	-0.18	0.16	-0.56	-0.39	0.30
11	8.475-8.825	0.44	0.04	-0.30	-0.66	-0.48	-0.24	-0.67	-0.32	-0.13	-0.29	-0.29	-0.04
12	8.925-9.275	0.23	0.08	-0.22	-0.44	-0.22	-0.11	-0.69	-0.16	-0.02	-0.23	-0.02	-0.08
13	10.25-10.95	0.48	-0.18	-0.48	-0.66	-0.36	-0.35	-0.70	-0.33	-0.25	-0.09	-0.12	-0.27
14	10.95-11.65	0.36	-0.35	-0.54	-0.55	-0.08	-0.30	-0.63	-0.15	-0.27	0.12	0.19	-0.42

* values written in bold are significant at P≤0.05.



Figure 2. Relationship between reflectance in spectral range 2.185–2.225 μ m and zinc concentrations in smelter waste barren of vegetation.

Table 2. Correlation coefficients between reflectance in 14 ASTER bands and selected chemical properties of smelter waste deposits covered with vegetation*.

Band No.	Spectral range [µm]	OM	Cd	Zn	Pb
1	0.52-0.60	-0.40	0.05	0.08	0.15
2	0.63-0.69	-0.48	0.48	0.33	0.43
3	0.78-0.86	0.63	-0.78	-0.89	-0.90
4	1.60-1.70	0.40	-0.40	-0.51	-0.59
5	2.145-2.185	-0.56	0.54	0.44	0.44
6	2.185-2.225	-0.50	0.35	0.36	0.31
7	2.235-2.285	-0.58	0.32	0.45	0.40
8	2.295-2.365	-0.68	0.48	0.55	0.54
9	2.360-2.430	-0.67	0.60	0.54	0.57
10	8.125-8.475	-0.69	0.58	0.66	0.68
11	8.475-8.825	-0.64	0.56	0.65	0.63
12	8.925-9.275	-0.55	0.61	0.55	0.54
13	10.25-10.95	-0.56	0.53	0.55	0.55
14	10.95-11.65	-0.48	0.46	0.49	0.47

* values written in bold are significant at P≤0.05.

case of surfaces with vegetative cover. Pb and Cd are elements of interest from practical perspective as these metals contribute to health and environmental risk in this area.

In a conclusion, we can say that our research provides a clear evidence that ASTER images hold a good potential for identification and spatial characterization of heavy metal variability in waste deposits present as hot spots in postindustrial areas. A semi-quantitative relationship between reflectance and metal concentrations exists in near infrared region for Cd, Pb and Zn for surfaces barren of vegetation, whereas short infrared region accounts for Zn variability in vegetated waste surfaces.

Combining traditional surveying methods with remote sensing enables for mapping of metal concentrations in waste deposits to tentatively delineate hot spots. Further testing and improvement of presented methodology is needed before its wider implementation.

REFERENCES

- Diersch H.-J.G., 2009. WASY Software FEFLOW 5.4 Finite Element Subsurface Flow and Transport Simulation System. Reference Manual, WASY Institute for Water Resources Planning and Systems Research Ltd., Berlin.
- Harbaugh A.W., McDonald M.G., 1996. Programmer's documentation for MODFLOW-96, an update to the U.S. Geological Survey modular finite-difference ground-water flow model. Open-File Report 96-486. U.S. Geological Survey. http://water.usgs.gov/software/code/ground_water/modflow/doc/ofr96486.pdf.
- Kemper T., Sommer S.R., 2002. Estimate of Heavy Metal Contamination in Soils after a Mining Accident Using Reflectance Spectroscopy. Environ. Sci. Technol., 36(12).
- Muzylo A., Llorens P., Valente F., Keizer J.J., Domingo F., Gash J.H.C., 2009. A review of rainfall interception modelling. J. Hydrolog., 370: 191-206.
- Niedźwiecki J., 2002. Hydraulic properties of A horizons of soils depending on the content of clay organic matter and bulk density. PhD Thesis, IUNG Puławy, 50 pp. (in Polish)
- Saulyev F.K., 1964. Integration of equations of parabolic type by the method of nets. New York: Macmillan Company.
- Soczyńska U., 1989. Hydrological processes. PWN, Warsaw. (in Polish)
- Terelak H., Stuczynski T., Piotrowska M., 1997. Heavy metals in agricultural soils in Poland. Pol. J. Soil Sci., 30: 35-42.
- van Genuchten M.Th., 1980. A Closed-form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils. Soil Sci. Soc. Am. J., 44: 892-898.
- Wangemann S.G., Kohl R.A., Molumeli P.A., 2000. Infiltration and percolation influenced by antecedent soil water content and air entrapment. Trans. ASAE, 43: 1517-1523.