

Water Quality at Catchment Scale



The research cluster "Water - Earth System Science" (WESS) - established in 2009 - focuses on the water cycle and associated solute fluxes at the catchment scale as a function of and in feedback with changes in climate, land use, and water usage. Of particular relevance is the fate of pollutants which are introduced by diffuse sources (atmospheric deposition, agricultural application, infiltration and continuous emission from urban areas). WESS is part of the German Water Science Alliance.

WESS is located on the campus of the University of Tübingen, Germany.





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WESS Research Outline



Goal and Scientific Objectives

The goal of WESS is to develop the capability of probabilistic quantitative projections of the water cycle and of water resources quality at the catchment scale in a changing environment, including:

- A profound understanding of the relevant individual processes in different environmental compartments, and a mechanistic and process-oriented description of these processes, including their interactions and feedbacks.
- A coordinated approach of model development, experimental investigations and process monitoring at the field scale.
- Assessment of uncertainties, e.g. via probabilistic modeling approaches, for improved interpretation of modeling results, on which management decisions rely.
- Model validations at well-characterized reference catchments.

Monitoring & Modeling Approach

The reliability of water and solute flux simulations depends on the quality of data fed into the models, on the representation of relevant processes, and on the accuracy of the numerical codes. High spatial and temporal resolution of the data is required for validating these models. Cost-efficient monitoring strategies and novel measurement techniques such as sensor networks and passive sampling devices are developed. Natural and anthropogenic compounds as well as isotopes can be utilized as tracers for the elucidation of origin, transport and reaction pathways of pollutants. The large amount of data needs to be processed using innovative data assimilation techniques. Finally, massive parallel codes have to be developed which can simulate reactive transport at the catchment scale for time periods of decades to centuries.

Such integrated numerical models are also a prerequisite to evaluate impact of management strategies and technologies.



Monitoring across scales

The Land Surface - Atmosphere Interface



The land surface and its feedbacks to atmosphere

- What are the evapotranspiration and groundwater recharge rates at catchment scale? How will they change in the future ? New model concepts considering non-equilibrium soil water dynamics, plant growth and root water uptake will improve the predictability of water fluxes at the land-surface
- How far do land-surface properties control climate at regional scales? The realization of high-resolution regional climate projections up to the convection-permitting scale will enhance the understanding of feedbacks between soil and vegetation processes and the atmosphere
- How to make meso-scale forecasts of extreme precipitation and flood events more reliable? Coupling hydrological and regional climate models via effective down- and upscaling algorithms for the variables to be exchanged between models acting at different scales will reduce uncertainties of runoff predictions



Observation of soil moisture, vegetation dynamics and flux rates of energy and water at the land surface.

Climate variability and land-use change can alter water and solute fluxes through the soil-plant-atmosphere continuum. In this context, a variety of science questions have still not been resolved such as how far water and energy fluxes at land-surface influence catchment hydrology and regional climate. To answer these and other related questions the working group focus on a better understanding of water and energy fluxes between vegetation and atmosphere and their feedbacks on regional climate.



Observed weekly means of latent heat fluxes (symbols, error bars) and corresponding simulations using the Community Land Model Clm3.5 (lines)

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The Groundwater - Surface Water Interface

The hyporheic zone is the transition zone between rivers and groundwater. It is a very dynamic and biologically active part of river catchments, plays a key role in the retention and transformation of water pollutants, and has the potential to provide important ecological services contributing to improving river water quality.

Quantifying the fluxes of water and solutes through the hyporheic zone and the transformation of compounds in this environment is of crucial importance to understand solute transport within river catchments. For this purpose, WESS follows a multi-disciplinary approach.



Modeled streambed geometry (upper panel) and model results (lower panel) of a 3D simulation of turbulent stream flow coupled to hyporheic flow and solute transport.

Schematic flow paths in the hyporheic zone, i.e. the transition zone between groundwater and river water.



- How much water flows through the hyporheic zone? Monitoring time series of physical, chemical and isotopic parameters allows to quantify amount, pathways and travel times of hyporheic exchange flows.
- What are the relevant biochemical processes? Studying interrelations between chemistry, organic matter and microbial communities provides information on the self-cleaning potential of rivers.
- What conditions favour pollutant degradation? Linking biochemical zonation and reactive turnover of pollutants are crucial for a general assessment and management of water quality.
- How can exchange flows for entire river reaches be assessed? Developing and applying reactive tracer techniques allows to assess the magnitude and time scale of hyporheic exchange flows across scales.



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Model Based Optimisation of Monitoring



- How to evaluate and optimize the design of monitoring strategies? Mathematical process models are combined with stochastic modeling tools and information-theoretic approaches to evaluate the worth of available data, the costs of additional data acquisition, as well as alternative monitoring designs.
- How to quantify and reduce uncertainty of model predictions? Holistic uncertainty quantification techniques trace the various uncertainty sources from the measurement procedure to the final model applications.
- How to assimilate different observation types in process models? A consistent land-surface-atmosphere data assimilation system obtains an improved estimate of the true state of the coupled system.
- How to derive continuous maps of soil and plant properties? A soil-landscape model utilizes techniques from pedometrics, geophysics, and remote sensing to obtain scalable spatial parameter fields for integrated catchment models.



(Left) Weather situation at 6UTC 2007 July 20th with colors indicating the equivalent potential temperature, a variable strongly linked to water vapor. (Right) Correlation between water vapor content and temperature (at ~1500 m a.s.l.) as considered by the EnKF-DART data assimilation system.

Innovative methods for uncertainty quantification across scales and for optimal design of monitoring schemes are developed and applied to coupled process models. Optimal design goals include reduction of model bias, uncertainty, and costs. Further, scalable soil-landscape models are developed to derive continuous maps of various soil and plant properties for improved parameterization of the models. These tools in combination with an integrated land-surface-atmosphere data assimilation and error quantification scheme opens up unprecedented opportunities for advancing integrated model understanding.



Uncertainty of groundwater level observations for predicting groundwater flow. Colors indicate potential uncertainty reduction in %.

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Physical & Chemical Monitoring

Numerous chemical compounds have been released into the environment by human activities (industry, agriculture, treated or untreated wastewater) and can nowadays be found in water, soil, and air at a global scale. Transport of these compounds is coupled to the water cycle.



Diurnal flux pattern of selected organic contaminants, released from a waste water treatment plant into the Ammer river.

- Which processes govern the long-term fate and transport of pollutants in the water cycle? The dynamics of solute transport are studied based on novel on-line measurements in stream water. Investigations in catchments contrasting in land-use, climate, and geology allows to elucidate relevant processes and impacts.
- Which compounds do accumulate in the water cycle? Analysis of persistent pollutants and their distribution patterns in soils, sediments, and biota give insight into legacy pollution. Comparing water chemistry at different times and locations allows the assessement of stability, turnover or accumulation rates of pollutants.
- How to assess dynamic groundwater recharge rates? A multiscale approach, depending on the required information content reaching from atmospheric observations to field-based investigations is applied for determination of soil moisture, vegetation parameters, etc. This also includes airborne and satellite remote sensing activities.



PCB concentrations in fish gave insight into a legacy pollution with PCB in the Ammer River.

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Multi-scale soil moisture monitoring infrastructure of the Schäfertal intensive research site.



Integrated Modeling at the Catchment Scale

WESS employs an integrated modeling strategy at catchment scale for simulation of the interactions and interdependencies of processes across the boundaries of environmental compartments.

The development of an appropriate modeling platform addressing the various spatial and temporal scales of processes in different compartments is a prerequisite for integrated models.



Ammer catchment with sampling points, streams and hydrogeological units.



Graphical user interface of OGS Data Explorer.

- Which processes govern the quality of ground- and surface waters at the catchment scale? A combination of process-based modeling (as a 'bottom-up ' approach) and multivariate statistics (as a 'top-down' approach) is applied to quantify processes controlling water quality at catchment scales.
- How can the transport and reactions of chemicals at the land surface, in the subsurface and in streams be represented in catchment models? Simplified models based on exposure times of solutes to various reactive zones in catchments are tested against complex 3-D reactive transport models.
- **How can we effectively parameterize integrated modeling approaches?** Innovative regionalisation strategies based on available maps, field data and remote sensing data are tested to better represent the spatial variability of catchment-scale transport processes.



Equipotential surface from a steady-state groundwater model and flow paths to groundwater production wells (left panel). Sampling of drinking water production wells to estimate groundwater age based on environmental tracer concentrations (right panel).

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WESS Collaborations and Links

- International Research Training Group (IRTG) "Integrated Hydrosystem Modeling" – a joint cooperation project of the Universities of Tübingen and Hohenheim with the University of Waterloo, Canada (http:// www.geo.uni-tuebingen.de/forschung/international-research-training-group-integratedhydrosystem-modeling.html).
- The Helmholtz Water Network coordinated by the Helmholtz Centre for Environmental Research, UFZ (http://www.ufz.de/watersciencealliance).

