Characteristics of main research directions investigated at the institute and the achievements 2010−2014

Institute	Institute of Hydrodynamics of the CAS, v. v. i.

The common orientation of the Institute is directed to hydrodynamic aspects of fluid mechanics. This comprises of analysis of laminar, transitional and turbulent flow regimes for both Newtonian and non-Newtonian fluids. A general description of all these flows is usually governed by the 3-dimensional Navier-Stokes equations (NSEs). In principle, the differences among the individual topics solved in the Institutes consist in the following entries:

- Significance of the individual members (or components of the corresponding vectors and tensors) in the NSEs subjects to the individual flow situations. From here it follows that some members can be neglected (analogously to Prandtl's considerations in the 40s'). It results in completely different initial forms of the reduced NSEs for the individual topics investigated in the Institute (Newtonian vs. non-Newtonian fluids, laminar vs. turbulent flow regimes, one-phase vs. multi-phase fluids, etc.).

- Initial and boundary conditions range from nearly exact forms to the approximate relations in not so strictly defined flows (e.g. strict defined geometry surrounding fluid flows vs. rainfall-runoff balance scenarios in hydrology).

- For the whole description of the different cases it is necessary to complete a continuity equation and balance equations by the so-called constitutive equation. This equation is not defined in a unique way which creates a lot of more or less successful proposals.

A consequent list of principal topics analysed in the Institute differs in the above mentioned items.

Modelling of flow behaviour of viscoelastic liquids by means of differential constitutive equations

Understanding the rheological properties of polymeric materials plays a key role for their processing. The rheological properties are subject to the molecular structure of the material and to the character of the flow. In principle, the character of the flow can be differentiated as shear or elongational (according to the type of deformation) and steady or transient (dependence on time). The rheological properties simultaneously generated by the material used and by the flow character are approximated by means of the constitutive models (equations). The total set of equations consists of the constitutive equations (CEs), momentum balance and mass conservation.

In the past three decades a number of differential and integral CEs have appeared capable to describe the complex rheological behaviour of viscoelastic materials. However, a decision which CE can be applied to which type of flow and material, and in which geometry is not so straightforward. This can be documented by the fact that in the literature there are contrary opinions of the physical importance of the non-evolutionary behaviour of rheological equations (influenced also by the stability of the numerical scheme).

At present, approximately six differential CEs are frequently used. These CEs differ not only in the individual members representing various physical entries but also in a number of parameters. However, two linear viscoelastic parameters (linear relaxation time and relaxation modulus) are common for all CEs, the remaining nonlinear so-called free parameters differ. To

describe the polydisperse viscoelastic materials more reliably, the discrete relaxation spectra are considered. Hence, each mode in a spectrum is characterized by its own numerical values of the entry parameters.

The frame invariant based Maxwell model is in its differential version known as the Upper-Convected Maxwell model (UCM). This model has no free parameter. The UCM model predicts constant steady shear viscosity η and first normal stress coefficient ψ_1 and zero second normal stress coefficient ψ_2.

The Giesekus constitutive model generalizes the UCM model taking into account anisotropic drag represented by a nonlinear coefficient α by means of which the shear thinning behaviour is governed. The Giesekus model predicts non-zero ψ_2. The elongational viscosity shows monotonic increase up to a constant maximum for $\alpha > 0$.

The PTT model respects the non-affine motion by introducing the Gordon-Schowalter derivative. The model assumes two forms - linear and exponential. Each form uses two free parameters participating in controlling the non-affine motion and governing shear thinning. The model predicts zero ψ_2. Its exponential version exhibits a maximum in steady elongational viscosity. For the non-affine motion, the unphysical oscillations in η and ψ_1 occur during a start-up of steady shear at higher rates.

The Pom-Pom model based on the idealised theory for branched molecules of H structure was consequently extended (XPP) by introducing the Giesekus term containing α, which allows to predict ψ_2. Both models (Pom-Pom and XPP) include two free parameters: stretch relaxation time and number of arms. Unlike the Pom-Pom model, the XPP model has one additional free parameter α linearly involved in the term participating in predicting ψ_2.

Both the original PTT and XPP models can be considered as special cases of the general network model (PTT-XPP) if the upper-convected derivative is replaced by the Gordon-Schowalter one and two terms are neglected. The PTT-XPP model uses the two identical free parameters as the Pom-Pom and XPP models and one additional free parameter resulting from replacing the upper-convected derivative by the Gordon-Schowalter one.

The Leonov model derived from heuristic thermodynamics arguments, results from the theory of rubber elasticity. It uses two free parameters depending on the relaxation time.

As is apparent from the above overview, a number of free entry parameters and their significance seems to be one of the crucial points in presentation of the individual models. The Institute has aimed to propose new CEs reducing a number of nonlinear parameters and simultaneously minimally preserve qualitative and quantitative characteristics in comparison with other differential CEs.

Nanoscale hydrodynamics for nano-particle systems

Properties of fluid flow in nanometre sized media may differ significantly from the flow in the classical media. As the medium through which fluid flows become smaller, the channel or particle surface plays a large role in impacting the flow properties through fluid-wall molecular interactions. For instance, the development of advanced membrane technologies with controlled and novel pore architectures is important for the achievement of more efficient and cost effective water and gas purification techniques, such as membrane distillation, reverse osmosis and CO_2 removal from natural gas. Membranes based on carbon nanotubes (CNTs) offer a possible route to overcome these shortcomings with a number of interesting structures emerging. CNTs are nanoscale cylinders of rolled-up graphene which have the outer diameter in the range of 1–3 nm. The fluid flow through a membrane composed of an array of aligned carbon nanotubes is four to five orders of magnitude faster than would be predicted from

conventional fluid-flow theory. This high fluid velocity results from an almost frictionless interface at the carbon-nanotube wall.

CNTs exhibit remarkable electrical and thermal conductivity, and are one of the strongest fibres known. These properties, combined with their nanoscale dimensions and large surface area have led to their intense study as prime material for gas and vapour adsorption. The electronic properties of CNTs are extremely sensitive to the chemical gas flow. Exposure to chemical environment dramatically influences the nanotube electrical resistance and thus electronic sensing which is commonly referred to as an electronic nose. Electronic noses were originally used for quality control applications in the food, beverage and cosmetics industries. Current applications include detection of odours specific to diseases for medical diagnosis, and detection of pollutants and gas leaks for environmental protection.

Nanoparticles are emerging also as a class of therapeutics for cancer treatment. Clinical results confirm that nanoparticle therapeutics show enhanced efficacy, while simultaneously reducing side effects, owing to properties such as more targeted localization in tumours and active cellular uptake. The application involving multifunctional nano-particulate systems combining targeting, imaging, diagnostics and therapy has the potential to detect diseases, deliver medications, and monitor the ability to change the current scenario of cancer research and diagnosis in real time.

Nanofluidics is the study and application of phenomena that involve fluid motion through or past structures with features that measure less than 100 nm in one or more directions. Consequently, the evolution of nanofluidic systems is accompanied by the emergence of new fluid phenomena which stem from interactions between the fluid and the walls of the nanofluidic systems and devices. The large surface-to-volume ratios influence the movement of fluids through hydrophobic nano-channels of nanofluidic devices used in separation processes and energy conversion. The surface charge dominates the electrokinetic flow behaviour in nanochannels, controlling the concentration of electrolytes and mechanical-to-electrical energy conversion by using pressure to drive a streaming current through the nanochannel. The development of nano-fabrication technologies now allow specifically designed nanofluidic devices to be fabricated. Simultaneously, the development of new instruments and tools for biotechnological applications, so called labs-on-a-chip, etc. which give the possibility of investigating fluid behaviour at the nanometre scale.

The interaction of suspended or fixed nanoparticles into the solid structure with fluids of industrial and biological character is decisive for a utility function of nanoparticles. The wide range of problems is in the scientific focus in the Institute including the molecular-level hydrodynamic analysis of interactions which enables to modify appropriately the contact surface of nanoparticles or to tailor their fixation into the solid structures and use them as a programmable membranes, detectors and nanofluidics for, e.g., cell analysis and separation of molecules.

Flow behaviour of electro- and magneto-rheological materials, electrospinning of polymer solutions

Magnetorheological (MR) fluids are multicomponent systems consisting basically of ferromagnetic particles usually within the size range of 100 nm–10 μm in diameter with high-magnetic permeability and low levels of magnetic coercivity dispersed in a non-magnetizable medium such as mineral oils or hydrocarbons. When a certain external static magnetic field is imposed, magnetic dipole and multipole moments are induced on each particle because of the multi-domain particle's structure. The anisotropic magnetic forces between pairs of magnetized particles promote the structuration into chain-like or columnar particulate structures aligned

with the direction of the magnetic field applied. Such internal structure development causes the liquid- to solid-like state transition in milliseconds, which is accompanied with the increase in viscosity within the MR fluids by several orders of magnitude and, hence, is able to support shear stresses resulting in large field-dependent viscoelastic moduli and a yield stress generation. The stiffness of MR structures may be further controlled via the magnetic field intensity. Moreover, the system returns to initially Newtonian-like fluid when the external magnetic field is switched off. Described field-responsive physical phenomenon ranks MR fluids among smart materials. Comparable behaviour can also be observed in electrorheological (ER) fluids, where external stimulus is external electric field. However, ER fluids do not exhibit appropriate values of the yield stress as well as viscoelastic moduli. Hence, at present the MR fluids are more commercialized systems providing applicability as various active damping systems, torque transducers, brakes and valve devices, shock absorbers, and elastomeric mounts.

The most significant problems of MR fluids are represented in poor long-term sedimentation and thermo-oxidation stability. Various techniques such as preparation of dimorphic particle-based suspensions and application of coatings of the particles with various materials are commonly used to prevent or suppress those drawbacks. Furthermore, poor stability of the bare particles under acidic conditions represents another well-known disadvantage requiring a corresponding attention.

The ER approaches analogous to those applied in the characterization of ER fluids can be also used in the case of electrospinning. In the electrospinning process, single jets are ejected from the apices of Taylor cones created at the surface of a drop of polymer solution. Jet forming is initialized by an electric field generated by a high-voltage power supply between the tip of the stick where the drop is stored and the grounded collector. In principle, the charged polymer jets are, during their passage from the tip onto the collector, simultaneously exposed to two basic factors reducing their diameters: high extension rate, the magnitude of which should not result in a jet disruption, and the rate of solvent evaporation optimally corresponding to the situation in which the solvent is completely evaporated at the moment of reaching the collector.

The Institute aims at magneto- and electro-rheological characterization of flow behaviour of the newly prepared materials reducing the above mentioned shortcomings. In the sphere of electrospinning the principal goal is in a basic pre-evaluation of suitability of the chosen materials for the process of electrospinning which should result in nanofibrous mats of good quality.

Coagulation of algal organic matter in water treatment process

The increased concentrations of algal organic matter (AOM) in raw water can seriously impair water treatment process efficiency and may even lead to the collapse of water treatment plan. The most pronounced adverse effects of AOM on drinking water production are the reduction in coagulation efficiency, membrane fouling, decreased adsorption efficiency for micropollutants and low-molecular weight compounds onto activated carbon, and disinfection by-product formation. AOM arises extracellularly through metabolic excretion as extracellular organic matter (EOM) or intracellularly during the cell lysis, forming cellular organic matter (COM). AOM is a mixture of peptides/proteins, mono-/oligo-/polysaccharides, lipids, amino acids and other organic acids of which proteins and polysaccharides comprise the majority. Consequently, the AOM composition can be characterised as protein and non-protein organic matter.

Coagulation is regarded as an effective technology when removing algae cells and hydrophobic and high-molecular weight organic matter such as humic acids. However, it is

widely accepted that if the organic matter in water is hydrophilic in nature, such as AOM, much lower removal efficiencies would be achieved. Several studies also showed that coagulation of AOM may be impaired by the formation of dissolved complexes between coagulant metals (aluminium and iron) and organics contained in AOM, especially proteins. This leads to an increase in coagulant demand and reduction in coagulation effectiveness. On the other hand, some studies observed a positive influence of high-molecular weight EOM as well as COM released after pre-oxidation on the coagulation of algae cells since algal biopolymers acted as a polymer coagulant aid.

Most of the investigations about the coagulation of algae-laden waters have focused on the removal of algal and cyanobacterial cells and some have also considered the influence of AOM on the coagulation of cells. Under certain circumstances, the amount of dissolved EOM and particularly COM can predominate over other impurities in source water. This happens during the die-off and decomposition of algal bloom. Studies on the coagulation of dissolved AOM in the absence of cells are very rare. Most of them investigated only the coagulation of EOM and their results are far from comprehensive. Furthermore, these studies, do not deal with coagulation of COM which may comprise a majority of dissolved organic matter in source water under circumstances described above. For these reasons, the following objectives of the institutional research were established: investigate the AOM properties, which are important from the perspective of coagulation, such as hydrophobicity, molecular weight, surface charge etc., isolate and characterise proteinaceous substances that were reported to disturb the coagulation process from COM of cyanobacteria, investigate the coagulation of peptides and proteins produced by *M. aeruginosa*, and to describe the coagulation mechanisms, quantify the contribution of the formation of dissolved complexes between peptides/proteins of cyanobacteria and coagulants (aluminium and iron) to the coagulation disturbance and to identify the peptides/proteins which are able to form dissolved complexes with coagulants and investigate the influence of peptides/proteins of cyanobacteria on the coagulation of kaolin particles which represent the clay particles (aluminosilicates) causing the turbidity of raw water.

Adsorption of algal organic matter onto activated carbon in water treatment process

Surface waters employed in drinking water production may contain a variety of organic pollutants of both natural and anthropogenic origin. Natural pollutants are generally recognized as natural organic matter (NOM) that are represented by humic matter (e.g. humic and fulvic acids) formed by the different ways of degradation and transformation of vegetable and animal materials in aquatic environment. Besides the humic matter, NOM involves algal organic matter (AOM) that is produced by phytoplankton and provides a significant contribution to the heterogeneous NOM mixture mainly in the summer season. In this period, water treatment plants often have to deal with increased concentrations of another important group of pollutants, especially pesticides of anthropogenic origin that get into the environment mainly from agricultural production. High concentrations of algal organic matter in the raw water may lead to low efficiency of coagulation and the related increasing consumption of coagulants. Other serious problems are membrane fouling, high formation of disinfection by products in chlorination and chloramination of waters with AOM, the production of taste and odour compounds, and harmful cyanobacterial toxins.

In terms of molecular weight (MW) distribution of coagulating AOM, the coagulation/flocculation processes are highly effective in removing organic molecules with high MW, whereas low-MW ones remain in the solution after the treatment. Some studies showed that cyanobacterial cellular organic matter (COM) peptides with MW < 10 kDa

represent residual dissolved organic matter (DOM) which is not supposed to be aggregated and separated during the coagulation in chemical water treatment. Therefore, other methods, such as adsorption onto activated carbon, need to be applied for their restriction.

The adsorption process using activated carbon, usually in the form of granular or powdered activated carbon, is frequently integrated in the drinking water treatment chain for removing undesirable organic impurities of both natural and anthropogenic origin. The vast majority of recent adsorption studies dealing with the removal of natural organic matter (NOM) is focused on humic and fulvic material or generally on dissolved organic matter and only a limited number of studies has addressed the specific adsorption of AOM. Analogous situation takes place in case of the simultaneous adsorption of natural (e.g. NOM) and anthropogenic organopollutants (e.g. pesticides, herbicides) which has been studied only for NOM of humic character, not for AOM. Hence, the negative effect of NOM and subsequent suppression of pesticide removal by activated carbon has been proved only for humic and/or fulvic acids due to their competitive adsorption. Based on the information mentioned above, especially the lack of adsorption studies dealing with the adsorption of AOM onto activated carbon or its competitive effect on adsorption of micropollutants, and the fundamental differences between properties of humic NOM and AOM (e.g. origin, composition, MW distribution, surface charge), the aims of the institutional research were as follows: to identify and then to separate the low-MW fraction of cellular organic matter produced by *M. aeruginosa* (namely peptides with MW < 10 kDa), which is hardly removable by coagulation/flocculation but it can be adsorbed onto activated carbon due to its specific properties, to characterise COM peptides < 10 kDa with respect to the properties affecting the adsorption (e.g. MW distribution, surface charge, content of functional groups), to quantify the adsorption capacity of selected adsorbents for peptide removal under different solution conditions, to identify AC characteristic affecting adsorption of AOM (e.g. pore size distribution, surface charge), and to evaluate the adsorption of organic micropollutants onto activated carbon (herbicides alachlor and terbuthylazine) and the competitive adsorption effect of COM products on their removal, to identify and then to describe the mechanisms and interactions acting in the adsorption of natural and anthropogenic organic pollutants onto activated carbon.

Vortical structures in transitional and turbulent flows

Flow investigation in terms of well-defined distinct structures still lacks generally acceptable definitions. By describing the flow in terms of vortical structures (or swirling motion), high-shear zones, or strain-dominated regions, different researchers will always get (at least slightly) different results. There is a clear need for universal criteria, as remarkably reflected in a long history of vortex identification. Various vortex-identification methods have been proposed during the last three decades. The search for efficient three-dimensional vortex-identification schemes has become particularly important for the analysis of transitional and turbulent flows, especially in the analysis of large-eddy simulation (LES) and direct numerical simulation (DNS) datasets. The understanding of vortex dynamics (i.e. generation, evolution, interaction, and decay of vortical structures) should be based on objective and unambiguous identification methods. There is no doubt that the physical reasoning for these schemes plays a crucial role.

There is an extensive amount of literature on vortex definition and vortex-identification techniques. Intuitive definitions often depict a vortex in terms of closed or spiralling streamlines or pathlines, local pressure minima, and isovorticity contours and surfaces. However, spiralling streamlines or pathlines are obtained just for an observer moving with the vortex to be identified, and the existence of a local pressure minimum does not guarantee the existence of a vortex (and vice versa). Vorticity tensor, as a Galilean invariant quantity (i.e. independent of

the translational velocity of an observer) expressing an average angular velocity of fluid elements, appears as one of the most natural choices for a vortex-identification criterial measure. However, it has been recently emphasized by many authors that vorticity is not suitable for vortex identification as it cannot distinguish between shearing motions and the actual swirling motion of a vortex.

Essentially, most vortex-identification schemes can be classified either as a region-type method or a line-type method. Without going into details, the objective of the line-type methods is to identify the vortex-core lines instead of general spatial regions. The region-type and line-type methods may be effectively combined as already shown in some previous flow-visualization studies. Although many of these region- or line-type methods are successful in vortex identification and provide valuable insight into various vortical flows, none of them has become universally applicable to all possible flow situations due to their specific limitations.

A vortex obviously represents a non-local flow phenomenon in space and time. However, the presence of viscosity in real fluids results in the continuity of the kinematic features of the flow field. Consequently, a reasonable estimate of some non-local vortical features can be inferred from the local (pointwise, applied point by point) characteristics and methods. The most widely used local methods for vortex identification are based on the analysis of the velocity-gradient tensor. It holds also for the recently proposed triple decomposition of the local relative motion near a point. The triple decomposition of motion is based on the explicit elimination of shearing motion. This decomposition technique results in two additive vorticity parts (and, analogously, in two additive strain-rate parts) of distinct nature, namely the 'shear' component and the 'residual' one. The residual vorticity represents a direct measure of the actual swirling motion of a vortex. However, this approach represents an optimization problem for each point in the domain, which makes the triple-decomposition method computationally relatively expensive.

In the Institute the following kinematic 'corotational' vortex-identification schemes were proposed and applied to various flow situations: (1) Search for a maximum of corotation of line segments near a point (given by the planar residual vorticity) over 'all planar cross-sections' going through the examined point; (2) The average-corotation method based on the proper averaging process applied to a set of all planar cross-sections passing through the given point.

The mathematical theory of the viscous incompressible Navier-Stokes equations

The Navier-Stokes equations (NSE) describe time evolution of the velocity and the pressure of viscous fluids. The regularity and uniqueness of solutions represent a key still unsolved problem: Do the solutions of NSE for incompressible fluids with smooth initial conditions and exterior forces stay smooth for all times or do they exhibit the so called blow-up at a finite time?

Although the mathematical theory of NSE has not yet been completed, some momentous results have been achieved in the last decades. There were specified some classes of functions, in which there exists only one weak solution. The problem of regularity and uniqueness was completely solved for some special cases and configurations: two-dimensional flows, axisymmetric flows, for the cases of small data and also on small time intervals. The so called large solutions have been intensively studied: their central idea is to specify wide classes of the ("large") initial conditions and exterior forces yielding global regular solutions. The definition of the so called suitable weak solutions was formulated and the existence of at least one such solution was proved for every configuration of the data. It was further proved that the 1-dimensional Hausdorff measure of the set of singular points of such a solution is equal to zero and this result has an essential impact on the study of the local regularity. Recently the conditional regularity has been intensively studied. The authors suppose that the weak solution

satisfies some additional properties and under such speculative conditions a full global regularity of solutions is then proved.

In the Institute the large time behaviour of solutions to NSE, which is closely connected with the problem of the regularity, was studied. There was discovered the phenomenon of the large time energy concentration: The energy of the solutions concentrates for large times only in some precisely described frequencies of the spectrum. Additionally, a close mutual relation between the structure of the initial conditions and the large time evolution of solutions was described.

Solid particles-liquid mixture flow

The common movement of solid particles and fluid in a mixture represents a comprehensive and important problem within fluid mechanics having many applications, represented e.g. by the sediment transport in channels, lakes and estuaries, hydraulic pipeline transport, flow in reactors. Particle movements in a mixture influence the fluid flow and reversely the fluid flow affects the movement of particles. Three types of interaction can be distinguished: particle-fluid, particle-particle (mutual), and particle-wall collisions. The energy of the liquid carrier keeps the solid materials suspended in the liquid stream and conveys them in the direction of liquid flow or pushes them along the conduit bottom in the form of a moving bed.

Solid-liquid mixture (slurry) flows can be classified in several ways related to the conveyed product according to its physical nature, carrier fluid or type of flow and one of the most common classifications relates to homogeneous, complex and heterogeneous (with particle saltation and sliding bed or stationary bed) flow patterns. Referred to as a non-deposit regime and regime with deposit, the fully-segregated flow regime (all particles are present in the bed layer) and the heterogeneous flow regime (flow with or without the bed and with heterogeneous suspension) can be differentiated.

Based on the conveyed material, we distinguish the *slurry with colloidal particles*, which behaves as a non-Newtonian liquid. The slurries with clay and dust particles (less than 63 μm) are called homogeneous or non-settling slurries and behave as homogeneous liquids, frequently of non-Newtonian behaviour. The particles are uniformly distributed within the conduit, differences between the particle velocity and the fluid velocity is negligible, and velocity and concentration profiles are nearly symmetrical. Pseudo-homogeneous and complex slurries contain fine and also coarser particles with significant settling tendencies, some segregation is evident and the flow is not axially symmetric.

If the mean particle diameter is greater than 63-100 μm, the flow pattern is heterogeneous. The heterogeneous slurries flow may be defined as flow with asymmetrical concentration and velocity distribution, particle conveyance as flow with a sliding bed and/or particle saltation and particle-wall friction of the Coulomb type contribution to the friction losses. Particles movement is realized in several modes: rolling, sliding, saltating and suspension, depending on the particle size, shape and density, flow conditions and conduit characteristics. In addition, the inertial effects of the particles must be taken into account since it usually outweighs the viscous effect of the slurry flow. In contrast to non-settling slurries the deposition-limit velocity is a very important parameter for complex and heterogeneous slurries; it is of the same importance as friction losses for design and operation.

Two main mechanisms of particle support, apart from buoyance force, are active in slurry flow – suspension by fluid turbulence and mechanical contact between particles (and between particles and wall of the conduit) - inter-granular contact stress. For small particles and relatively large velocities, turbulent suspension is dominant, and the particles are distributed relatively evenly throughout the pipe.

In recent years, more attention has been devoted to the investigation of high concentrated (dense) homogeneous and pseudo-homogeneous slurries including modelling and measuring of their internal structure. A majority of the research has been done for non-settling slurries rather than for heterogeneous and complex slurries. Stratification is due to settling of coarser particles in a sheared carrier resulting in the formation of a sliding or stationary bed along the pipe invert. It should be mentioned that the classification into settling and non-settling slurry reflects only extremes in the continuous spectrum of the slurry behaviour.

Recent investigations of settling-slurry did not well enough recognize the internal structure and mechanism of the slurry flow, they were conducted mostly with respect of integral characteristic only, and understanding of settling-slurry flows and knowledge about the slurry flow structure are relatively poor to develop the physically based predictive models.

The knowledge of the slurry flow behaviour and the control of its inner structure make it possible to optimise the energy and water consumption, to improve quality, safety and reliability of the slurry transport and processing, and industrial exploitation of the slurry flow, i.e. hydraulic pipeline transport can benefit from the research results.

The Institute particularly focussed on the flow of homogeneous and complex dense slurries in pipe, laminar / turbulent transmission, effect of mechanical treatment and drag additives on pressure drop reduction and slurry flow behaviour, heterogeneous slurry conveying in horizontal, inclined and vertical pipes and the effect of particle size distribution.

Variability of hydrological cycle components in changing environment

The hydrological cycle and water management represent a domain seriously endangered by climate change. In recent years, the regional climate models (RCMs) were established as an essential tool in climate research, translating large-scale information from global climate models to the regional scale. Their outputs are submitted to hydrological models in order to investigate the impact of potential climate change on water resources.

The spatial resolution of the RCMs is too coarse to capture some physical processes influencing the local climate. This results in the systematic deviation of model outputs from the observed data. The daily precipitation time series, which are the crucial input to the hydrological studies, belong to the most affected variables. Hence, a bias correction of the data is necessary prior to their usage in impact studies. Several correction methods were elaborated on and applied to daily precipitation sums as power transformation or quantile mapping. Nevertheless, validity of these methods is affected by a non-stationarity of the precipitation time series between the calibration and application, which causes a certain degree of uncertainty in the following research.

Traditional hydrological models have concentrated on catchment scale rainfall-runoff predictions, thus avoiding the complexities of local scale hydrological mechanisms. Recently, mesoscale distributed hydrological models represent a promising tool which might investigate the spatially variable impact of climate change. This is especially the case regarding the information about the soil water regime. Insight into internal hydrological processes governing the overall soil water regime, such as rainwater infiltration, soil water retention, evaporation, water uptake by plants (transpiration), surface and subsurface runoff formation, is needed for credible predictions of the hydrological effects of the changing climate. This could be achieved by analysing long-term meteorological and hydrological time series as well as by analysing individual short-term hydrometeorological events including high-impact precipitation events and drought events. The insufficiency of existing long-term observation data sets is often reported (they tend to be inhomogeneous, suffering from insufficient spatiotemporal resolution, and loaded with high uncertainty due to measurement errors) and thus short-time studies are

supposed to be relevant for the description of hydrological processes especially in small basins. Especially mountainous headwater catchments provide unique opportunity for studying water regime of different hydrological compartments and energy and transport processes at detailed temporal scales. They are highly sensitive to climate stress, and also characterized by distinct seasonality and high inter-annual variability of winter and summer conditions. These headwater catchments play a major role in initial stages of large-scale flood events and also higher frequency of flash floods is known to occur in the mountainous regions. In both humid and arid climate, headwater catchments serve as important sources of drinking water.

The existing hydrological research of the Institute has been focused on: (i) long-term hydrological modelling using the long-term observation data sets in order to describe water regime under the climatic changes; (ii) improved quantitative understanding of processes controlling the transfer of water and heat near the land surface, including soil-plant-atmosphere interactions. For the purposes of the above-mentioned scientific lines the network of environmental observatories and headwater catchments created and operated by the Institute has been utilized. Special attention has been paid to the soil profile as an important part of the hydrological cycle and attempts were made to describe the soil water regime, heat transfer and water uptake by the plant root system (transpiration).

Research Report of the team in the period 2010–2014

Institute	Institute of Hydrodynamics of the CAS, v. v. i.

Scientific team	Hydrodynamical Aspects of Fluid Mechanics

Constitutive modelling of flow behaviour of polymer melts, measurement of elongational viscosity

Constitutive models complete the set of balance equations describing the flow of polymer melts. A phenomenological modification of the eXtended Pom-Pom (XPP) model was proposed with the aim to reduce the number of free non-linear parameters. The modified XPP model includes three parameters per mode in total (two linear viscoelastic parameters - linear relaxation time λ and shear modulus G, and one non-linear parameter). The original XPP model contains five parameters (two linear viscoelastic parameters and three non-linear ones, one non-linear parameter participates in the second normal stress difference prediction). The predictive/fitting capabilities of the modified model were compared with the Giesekus, XPP, and modified Leonov models using various low-density polyethylene materials in steady and transient shear and uniaxial elongational flows. It was found that the modified model is capable of predicting/fitting the rheological properties (not second normal stress difference prediction) for studied low-density polyethylene materials with sufficient accuracy, including strain hardening in uniaxial elongational flow.

Constitutive models should respect objective thermodynamics and stability conditions ensuring their validity in the whole range of possible deformation flow. However, in practice a very good description of flow situations can be achieved with the models not complying with the physical assumptions in all respects. Analogously to the term characterizing yield stress in empirical viscoplastic models, the term represented by the Gordon-Schowalter (GS) derivative in the differential constitutive models contributes to better fitting the experimental data, especially shear thinning. Efficiency of the above stated modified XPP model (just one non-linear parameter per mode) implementing the GS derivative term (one additional non-affine motion parameter per mode) is improved (documented among others on low- and high-density polyethylenes), and a favourable comparison with the exponential Phan-Tien-Tanner (PTT) and PTT-XPP models (a priori containing the GS derivative term) was carried out.

For responsible testing of the individual constitutive equations, the sufficiently precise experimental data of elongational viscosity are necessary. However, the measurement of elongational viscosity still evokes a series of problems in comparison with the relatively well-established measurement of shear viscosity. A Sentmanat Extension Rheometer (SER) represents one out of a few experimental devices for the measurement of elongational viscosity of polymer melts. However, the appropriateness of this technique for individual polymer materials is not sufficiently apparent and in some cases is disregarded or ignored. The proposed visualization technique was based on imprinting painted pattern from the inner surface of the studied polymer samples onto the counter-rotating drums. Digitization of the imprinted pattern gives a possibility to evaluate a degree of sagging, incorrect fixing of rectangular polymer samples to the drums, possible appearance of sample inhomogeneity (variance in thickness, bubbles, etc.). The presented visualization technique was demonstrated using branched low-density polyethylene materials. Two various imprinted patterns were applied. First, the upper

and lower contours are charted on a prepared sample with the aim to determine the sample shapes during stretching and to compare them with the theoretical ones. Second, the inclined rectangular grid pattern is charted for evaluating possible inhomogeneity of the sample. This method enables to categorize the individual materials with respect to the applicability of the SER device.

Gas adsorption and permeation through nano-composite films based on a deformable entangled network of carbon nanotubes

The aim was to prove that the entangled carbon nanotube (CNT) network structures have a great potential for developing high-performance polymeric composite materials in terms of the compressive and tensile deformation, the control of rheological behaviour, the gas and chemical vapour permeation and adsorption/desorption properties affected by CNT chemical functionalization. It was found that the macroscopic entangled CNT structure can proportionally transfer unique properties of CNT into composites and bring substantial improvements in electrical and thermal conductivity, sensing of organic vapours and control of the permeation rate by an electric current.

The link of rheological properties of polymeric nano-composites with electro-conductivity proved to be useful in case of the measurement of longitudinal and compressive deformation of CNT network/polyurethane composites. The composite was prepared in an original way taking a non-woven polyurethane filter membrane and enmeshing it with carbon nanotubes. Testing has shown that in this way prepared composites can be extended as much as 400 % during which the electrical resistance increases more than 270 times. When the compression has been applied to the composite, the compressive strain increased up to 25 %. As an example of the composite use as a strain sensor, a human knee flexion has been tested, that may, for example, be useful in orthopedics and rehabilitation.

To model the mechanical behaviour of polymer nano-composites, a nonlinear rheological model was proposed as a combination of the elastic and the friction stresses with a kinetic equation. The network of entangled multiwall carbon nanotubes, which is the filling part of the composite, is an assembly of non-bonded and randomly oriented units whose mechanical behaviour is affected by their buckling, compression and slippage at contact points. Slippage and irreversible nanotube rearrangements were evidenced by the hysteresis in the stress-strain curves during loading and unloading cycles and longitudinal deformation. Accordingly, the model of the composite rheological behaviour described mainly the nanotube bending in compression and the nanotube slippage at the contacts points.

For the first time it was shown the increase of permeation rates of some volatile organic compounds through CNT networks by an electric current. The change in the permeation rate is reversible when the current is turned off. The permeation rise was partly probably due to Joule effect and thus increased membrane temperature and vapour pressure in the vicinity of the inlet side of membrane. However, the effect of vapour polarity and electrostatic interaction of vapours and charged nanotubes were also involved.

The sensitivity of pristine and functionalized CNT networks and CNT network/polymer composites to various alcohol and hydrocarbon vapours was investigated by the resistance measurement. The vapours had different polarities given by Hansen solubility parameters and different volume fractions of saturated vapours defined by the vapour pressure. The results revealed that the network electrical resistance increase depends on the polarity of vapours and particularly, on diamine functionalization of nanotubes. The influence of diamine modification on interaction between the nanotube network and vapours enhanced the network sensitivity as much as thirty times in comparison to the sensitivity of pristine nanotubes. The possible

mechanism of this sensitivity increase was revealed from the Fourier transform infrared analysis, that is, the enhanced vapour sensor response can be attributed to the extent of the interaction area between the carbon nanotubes and vapours.

Electro- and magneto-rheological behaviour of smart materials, electrospinnability of polymer solutions

Change of rheological behaviour of electro (magneto)-rheological materials in electric (magnetic) field ranging in full scale from liquid- to solid-like consistency gives many innovative applications in various industrial branches. However, a usage of metallic nano- or micro-particles in Newtonian carrier liquids usually deteriorates stability of rheological characteristics of these materials in time. The adverse factors as e.g. sedimentation and corrosion can be substantially reduced by creating polymer shells round the particles. On the other hand, these core-shell structures cause worsening of electro (magneto)-rheological phenomenon. A series of rheological measurements in shear and oscillatory regimes was carried out in the presence and absence of the electric (magnetic) field with the aim to evaluate pros and cons of the above introduced surface covering of the nanoparticles. Based on these measurements it was possible to evaluate perspective electro (magneto)-rheological materials for which a reduction of electro (magneto)-rheological phenomenon has negligible impact to possible industrial usage; on the contrary an improved time stability non-negligibly contributes to their applicability.

From here it follows that electrorheological measurements represent a key approach in characterizing the efficiency of electrorheological fluids. The rotational rheometers, the Physica MCR 501 (Anton Paar Co.) equipped with an electrorheological cell and the Bohlin Gemini CVOR 150 (Malvern Instruments) modified for electrorheological experiments, generate an electric field in two completely different ways. Each of the two generations has a specific influence on electrorheological measurements. The experimental data were obtained and compared for a suspension of polyaniline powders mixed (10 wt.%) in silicone oil. For a concentric-cylinders arrangement, it was shown that the data are fully comparable for both rheometers. However, for a parallel-plate arrangement, the data using the MCR 501 provide higher values in comparison with both the corresponding plate-plate data obtained with the Gemini CVOR 150 and with the mutually comparable concentric-cylinders data.

During the process of electrostatic spinning, the rheological behaviour of polymer solutions is significantly influenced by the presence of an external electric field. The aim was to find a correlation between the electrorheological characteristics of polyvinylbutyral (PVB) solutions and their electrostatic spinnability. When exposed to an external electric field, PVB solutions with either poor or good solvents respond in different ways. It was shown that the complex viscosity ratio η_E^*/η_0^* (where η_E^* and η_0^* represent complex viscosities of a solution in the presence and absence of an external electric field, respectively) can serve as an indicator as to whether a chosen material is a potential candidate for an acceptable electrospinning process. This occurs when the ratio η_E^*/η_0^* increases with an increasing electric field strength, i.e., when poor solvents are applied. The possible changes to the physical and chemical properties of PVB solutions were investigated using scanning electron microscopy (SEM), Fourier transform infrared spectroscopy (FTIR) and differential scanning calorimetry (DSC) techniques.

The quality of electrospun fibres is subject to many factors ranging from the characteristics of the materials used to processing conditions. Although an important parameter for applicability, less attention has been paid to the storage stability of applied polymer solutions and its impact on the quality of electrospun webs. The aim was to analyse the storage stability

of polyvinylbutyral solutions in methanol and ethanol for the formation of undisturbed nanofibres. The quality of nanofibrous mats produced over a period of 197 days, during which the solutions were stored under constant conditions, was investigated. Using rheological measurements, SEM, FTIR, and DSC techniques, it was shown that the storage period for the solutions used had almost no influence on the quality of electrospun fibres, which is a positive result for practical use.

The influence of algal organic matter on water treatment processes

Algae are ubiquitous in rivers and reservoirs supplying drinking water treatment facilities. When algal populations increase in these reservoirs, which happens especially during summer season, water treatment technology has to deal not only with increased cell concentration but also with dissolved algal organic matter (AOM). It arises extracellularly via metabolic excretion, forming extracellular organic matter (EOM) or intracellularly due to cell lysis, forming cellular organic matter (COM). COM is released during the population growth and decline and also during the water treatment process if pre-oxidation methods, inducing the cell rupture, are used. The highest concentrations of dissolved AOM are present in raw water after the collapse of an algal bloom in the form of COM released from damaged cells.

The increased concentrations of AOM in raw water can seriously impair water treatment process efficiency and may even lead to the collapse of water treatment plant. The most pronounced adverse effects of AOM on drinking water production are the reduction in coagulation efficiency, membrane fouling, decreased adsorption efficiency for micropollutants and low-molecular weight (MW) compounds onto activated carbon, and toxic disinfection by-product formation. For these reasons, the following main objectives of the research were established: (i) Investigate the AOM properties, which are important from the perspective of coagulation, such as hydrophobicity, molecular weight, surface charge etc., (ii) investigate the coagulation of AOM produced by cyanobacteria, and to describe the coagulation mechanisms, and also investigate the influence of AOM on the coagulation of kaolin particles which represent the clay particles (aluminosilicates) causing the turbidity of raw water and (iii) identify the peptides/proteins of *M. aeruginosa* which are difficult to remove by coagulation and to present another process which may be effective in removal of these peptides/proteins.

The results achieved are summarized as follows:

The AOM of the three cultivated algal species (*Microcystis aeruginosa*, *Fragilaria crotonensis* and *Chlamydomonas geitleri*) is predominantly hydrophilic, with low SUVA (Specific UV Absorbance) and significant portion peptide/protein material that is most noticeable in COM of *M. aeruginosa*. The AOM composition and characteristics is species-specific and change with the growth phase. EOM and COM show several differences. Specifically, a portion of peptides and proteins, protein quantity and diversity, a portion of hydrophilic fraction and of high-MW compounds are significantly bigger in COM than in EOM. On the other hand, COM has lower SUVA than EOM. EOM and COM of all three species contain large portions of low-MW (< 1 kDa) compounds and high-MW (> 100 kDa) polysaccharides. Peptides/proteins exhibit narrower MW distribution than non-peptide fraction and it widen as the cultures grow.

Coagulation of peptides and proteins is strongly dependent on pH value and on the charge properties of the involved particles/molecules. The highest coagulation efficiencies (between 60 and 85% depending on initial concentration of peptides and proteins) are achieved at acidic pH values (pH 4 - 6 for ferric coagulant) due to electrostatic interactions between positively charged Fe-hydroxopolymers and negatively charged functional groups of peptides/proteins.

4

At low COM peptides and proteins/coagulant ratio (e.g. w/w DOC/Fe = 0.14), adsorption of peptides/proteins on the surface of colloidal Fe-oxide-hydroxide particles at pH values 6 - 8 may also be an important coagulation mechanism. On the other hand, when peptides and proteins/coagulant ratio is higher (e.g. w/w DOC/Fe > 0.43), the surface of Fe-oxide-hydroxide particles becomes completely covered with peptides/proteins, which leads to an increase in the negative charge density as peptides/proteins bear a significant amount of negative charge at pH 6 - 8 and to a charge stabilization of particles. When COM peptides/proteins occur in turbid waters, optimum pH values for effective treatment substantially change. At pH values suitable for the removal of kaolin (7 - 8.5 for Al and 6.4 - 8 for Fe coagulant), poor removal is achieved in the presence of peptides/proteins and the optimum pH for coagulation of peptide/protein-kaolin mixture decreases to pH 5 - 6.5 for Al and 4 - 6 for Fe. At these pH values, electrostatic interactions between amphoteric peptides/proteins, negatively charged kaolin particles and positively charged coagulant hydroxopolymers enable coagulation. Peptides/proteins interact electrostatically with kaolin even in the absence of a coagulant, but they coagulate only at quite low pH values (pH < 4.5), and lower removal rates for DOC (about 45%) compared to tests with Al/Fe coagulants are achieved. It was also shown that AOM peptides and proteins deteriorate the coagulation process by formation of dissolved complexes with coagulants (both Al and Fe dissolved species). However, this happens at quite narrow pH range (about 6.8 for Al and 6 for Fe) and can be avoided by optimization of pH conditions. Peptides and proteins of apparent MWs of approximately 1, 2.8, 6, 8, 8.5, 10 and 52 kDa are responsible for formation of complexes. The maximum capacity of peptides and proteins to bound iron was observed to be about 1.2 mmol Fe per gram DOC. Results confirmed that high-MW proteins (apparent MW > 10 kDa) are easily removable by coagulation, whereas low-MW peptides (< 10 kDa) are removed very poorly. Other treatment techniques need to be employed for their removal, particularly considering that they may include cyanobacterial toxins.

It was shown that non-coagulated low-MW peptides may be removed by adsorption onto activated carbon (AC). The peptide adsorption onto activated carbon is highly pH dependent and increases with decreasing pH value. The highest adsorption capacities were reached at pH 5 due to the electrostatic attraction between functionalities of the AC and the peptides and/or thanks to the conformation changes in the structure of peptide molecules. Furthermore, a high portion of secondary micropores and mesopores in AC structure contributes to the peptide removal because these pores provide a fundamental portion of the specific surface area available for adsorption of natural polymers with MW < 10 kDa. Adsorption experiments at different electrolyte concentrations demonstrated that ionic strength significantly impacts the adsorption of organic pollutants. In case of the peptides, an increasing ionic strength can enhance their adsorption by screening the repulsive forces, or by strengthening the attractive ones in the adsorption system, all of that depending on the type of carbon used and pH applied. The characterisation of COM properties important in terms of adsorption showed that peptides have an amphoteric character and contain different functional groups, e.g. –OH, –COOH, –SH, $=NH_2^+$, $–NH_3^+$. Thanks to de-/protonation of the ionizable groups, COM peptides carry both positively ($=NH_2^+$, $–NH_3^+$.) and negatively charged sites ($−COO^-$) which enable the existence of electrostatic interactions with charged groups on carbon surface during the adsorption. In addition to van der Waals forces and hydrophobic interactions that are the driving forces for adsorption onto AC, a formation of H-bonds and electrostatic interactions were confirmed to play an essential role during the removal of organic pollutants onto activated carbon.

Vortical structures in transitional and turbulent flows

Unsteady flow nature of vortical structures in transitional and turbulent flows makes their identification, characterization, and analysis a rather complex problem which was investigated in detail.

Controversial aspects of the conventional and widely used concept of the integral vortex strength were treated in detail. The strength of a vortex is usually calculated (for a planar cross section) as the circulation along the vortex boundary, or equivalently due to Green's theorem, as the surface integral of vorticity over the planar vortex cross section. However, the local effect of an arbitrary "superimposed shear" is fully absorbed by vorticity what makes the circulation a shear-biased integral characteristic. It was shown that different vortex-strength models can be derived on the basis of different local vortex intensities proposed in the literature. The outcome of these models naturally differs, even for an ideally axisymmetric vortex. Three different vortex-strength models were compared and discussed by examining the unsteady Taylor vortex.

The recently proposed vortex-identification scheme based on the triple decomposition of the local motion (triple decomposition method, TDM) considering the local motion near a point a superposition of three elementary motions – straining, shearing and rigid-body rotation – was successfully applied in 3D vortex identification. Accordingly, the vorticity portion associated with the rigid-body rotation (the so-called residual vorticity obtained after the elimination of local shear) was employed as the new vortex characteristic.

A new kinematic measure of local vortex intensity near a point was introduced and employed in 3D vortex identification. It is based on the maximum corotation of line segments found within a set of planar cross-sections going through the given point. The results obtained at higher thresholds for different vortical flows were promising. The proposed kinematic method remains applicable to compressible and variable-density flows. This approach was further extended: An easy-to-interpret kinematic quantity measuring the average corotation of material line segments near a point was introduced and applied to vortex identification. At a given point, the vector of average corotation of line segments is defined as the average of the instantaneous local rigid-body rotation over "all planar cross sections" passing through the examined point. The vortex-identification method based on the average corotation is a one-parameter, region-type local method sensitive to the axial stretching rate as well as to the inner configuration of the velocity gradient tensor. The method was derived from a well-defined interpretation of the local flow kinematics to determine the "plane of swirling". It is applicable to compressible and variable-density flows. Practical application to direct numerical simulation datasets includes a hairpin vortex of boundary-layer transition, the reconnection process of two Burgers vortices, a flow around an inclined flat plate, and a flow around a revolving insect wing. The results agreed well with some popular vortex-identification methods and performed better in regions of strong shear.

A comparison of implicit and explicit shear-eliminating vortex-identification schemes was performed. The explicit ones are represented by the TDM and by the average-corotation scheme. Four different flow situations were analysed in terms of the two explicit shear-eliminating schemes and two standard implicit criteria: Q and lambda-2. It was shown that explicit shear-eliminating methods are more efficient in regions of strong shear than the implicit ones.

Large time behaviour of global turbulent solutions to the 3D Navier-Stokes equations

The time evolution of global turbulent solutions is an integral part of the mathematical theory of the Navier-Stokes equations (NSE). The most conspicuous feature here is the time decay of the solutions for the equations without a forcing term which can be measured in the norms of various spaces. This decay is studied both locally and for time going to infinity. We showed that the decays in time of solutions measured in suitable graph norms locally on short time intervals are always bounded along the whole trajectory of the solution. Surprisingly, the energy of the solution concentrates in the long run in small and possibly middle frequencies. Consequently, no solution decreases more quickly than exponentially. The results hold for a wide class of three-dimensional domains including domains with non-compact boundaries.

Global turbulent solutions to NSE in the whole three dimensional space exhibit some special properties. Additionally to the properties mentioned in the previous paragraph the decays in time of any space derivative of an arbitrary order on short time intervals are always bounded along the whole trajectory. In the long run the energy of the solution concentrates in the frequencies from an arbitrarily narrow annulus or in an arbitrarily small ball in the Fourier space. As a result, the energy of the solution decreases either exponentially or algebraically. By the use of the Fourier transform it is possible to describe the rate of disappearance in time of high frequencies.

Another striking feature of the large time behaviour of solutions is a close relation between the structure of initial conditions − which is described by the use of suitable Besov spaces − and the long-time evolution of kinetic energy of solutions to NSE. We presented a precise mathematical description of the dependence of the rate of the long-time energy decay on the distribution of frequencies in the associated initial conditions. The relation between the structure of initial conditions and the rate of the energy decay is not impaired by a potential turbulence of the flow: the results hold for all turbulent solutions. For the case of forced NSE with a time dependent external force the situation is more complicated. Surprisingly, the energy can be asymptotically distributed over the entire spectrum of the Stokes operator regardless of the structure of the initial conditions and the external force. Nevertheless, there exists a wide class of initial conditions and external forces yielding solutions with the large-time energy concentration analogical to the situation in the unforced NSE.

Solid particles-liquid mixture flow

The effect of particle size distribution, average slurry velocity and concentration on the pressure drops, slurry flow behaviour and its structure was studied for selected homogeneous, complex and heterogeneous particle-liquid mixtures. Experimental results were evaluated and compared with theoretical and predictive models and suitable models were suggested for individual mixtures and flow conditions.

It was confirmed that the flow of homogeneous (e.g. kaolin) and complex (e.g. sand) mixtures depended strongly on the contents of colloidal or dust particles and slurry physico-chemical properties. These mixtures can be described by the Herschel-Bulkley or Bingham models in the laminar region, and by the Wilson or Slatter models in the turbulent region. All the above mentioned models are suitable even for scaling up.

The flow behaviour of fine-grained mixtures is controlled by the attractive and repulsive forces between the particles given by the physical and chemical properties of the solid and liquid phases. Peptization or mechanical treatment resulted in a significant decrease in the yield

stress, apparent viscosity, the pressure drops and velocity of the laminar/turbulent transition, which was accompanied by a high level of flow instability and pressure fluctuations.

Flow behaviour of heterogeneous mixtures depends on particle size distribution, density, shape and concentration, and on properties of the carrier liquid. The effect of particle size depends on the flow velocity. The addition of fine particles (e.g. kaolin) favourably affected the flow behaviour and pressure drops of the sand-water mixtures, similarly as addition of coarse particles to fine-grained mixtures.

The coarse particle–water mixtures were significantly stratified, for moderate and higher flow velocities the saltation became a dominant mode of the particle movement. Bottom formations (dunes) or bed layer were frequently formed in the horizontal pipes for lower flow velocities and /or concentrations. The relative high slip velocity, particle-particle and particle-pipe collisions resulted in significant increase of the pressure drops.

The velocity profiles of the carrier liquid and conveyed particles were evaluated by the PIV method for movable and stationary bed, and the trajectories of particles were determined. The flow over the dunes was simulated using the finite element method. The shapes of dunes observed through a transparent pipe section were used as the boundary conditions for the numerical simulations. The dunes velocities equalled the erosion velocity and were several times lower compared to the particle velocities; it significantly decreased transport concentration for low mixture velocities. Good correlations between pressure differences determined from the simulations and the experiments were achieved.

The frictional pressure drops in the vertical pipe were found to be less than those in the horizontal pipe due to the fact that the contact load produced significant energy losses. The frictional pressure drops were not significantly influenced by the pipe inclination, the maximum pressure drop was reached for pipe inclinations from 20 to 40 degrees in ascending pipe section in dependence on concentration and flow velocity.

The concentration distribution was measured using the gamma-ray densitometers. Nearly linear concentration distribution was recognized in the central part of the pipe, and its slope slightly decreases with increasing mixture velocity. Evaluated from the concentration maps was a real in situ concentration and it was confirmed that transport concentration in a horizontal pipe increased with increasing flow velocity. The different concentration distribution patterns were observed in ascending and descending pipe sections.

Mutual interactions of the particles and carrier liquids were numerically analysed using the lattice Boltzmann method (LBM). Efficiency of this analysis was documented by comparison with experiments where the trajectories and velocities of the particles were measured in a conduit of width 40 mm where the bed was covered by stationary spherical particles of the same size as the moving particles. It was shown that the LBM simulation is able to reproduce adequately physical behaviour of real particles and thus can contribute to a better understanding of the particle-fluid dynamics. Moreover, the developed simulation allows examining various initial and boundary conditions otherwise difficult to prepare experimentally and thus it can also serve as a guide for the design of prospective experimental setups.

Experimental observations and numerical simulations were performed on the model of a separator of swirl geometry in a scale 1:10 with the aim to study efficiency of solid particles deposit. It was shown that the numerical simulations (Finite Volume Method + Discrete Element Method) can reasonably predict the flow field inside the separator only in a case when no bottom outflow is considered.

Variability of hydrological processes in changing environment

In the field of bias correction of the climate model data, attention was paid to deriving methods reducing an influence of the non-stationarity. The main idea was based on the fact that the simpler relations with a reduced number of parameters are more resistant against errors caused by non-stationarity in comparison with the more precise and more complex transfer functions. Two new correction methods based on an analysis of the gamma distribution were obtained. The comparison with the quantile mapping as the most frequently used method indicates their better applicability in non-stationary conditions.

The semi-distributed hydrological model SWIM was utilized with the aim to estimate the impact of the climate change on the water resources in the Czech Republic. The particular components of the hydrological cycle were compared with the observed data. The discharge, groundwater level and evapotranspiration estimates were validated using two mesoscale catchments with various natural conditions (mountainous forested and lowland agricultural). The efficiency of the soil water content module was investigated and contrasted with another approach in a small-scale experimental area. The results confirmed the assumption that the SWIM model is reasonably capable of simulating all tested variables in both catchments. Nevertheless, several uncertainties were described (e.g. winter soil moisture content and snowmelt estimation).

The climate change impact investigation showed that the most significant change in discharges takes place in the spring period. Due to a precipitation translocation to the winter period and increasing temperature, the snowpack is expected to be lower and thus the spring discharges drop significantly. Summer discharges have also decreased, but the magnitude was lower than in spring. The soil moisture content has dropped most profoundly in autumn. The winter period characteristics, concerning discharge, evapotranspiration and soil moisture, seemed to be almost unaffected by the climate change. Also a simulation of the future runoff regime in small forested headwater catchments showed a shift towards the higher incidence of extreme hydrological situations, and decreases in runoff in the summer and autumn months. At the same time, however, an increase in the frequency of flooding caused by torrential precipitation is predicted.

The water exchange between soil and plant roots was studied and described using a simple macroscopic, vertically distributed plant root water uptake approximation adopted and implemented in a model of soil water flow based on the Richards' equation. This combined model was used to simulate soil water movement at a forested site in a small headwater catchment. The results were compared with observations (sap flow, soil water pressure, and soil water content). Soil thermal conditions during the vegetation season were simulated using a dual-continuum model of coupled water and heat transport in the same mountainous region. The soil heat flux simulation results are greatly influenced by the depth of the soil profile and by the bottom boundary condition applied. It was found out that the soil thermal conditions are strongly affected by the root water uptake that not only affects the temperature of the water withdrawn but also controls the soil thermal conductivity near the soil surface. Additionally the impact of forest canopy on snow cover characteristics, rain interception and separation of the runoff using of the natural tracer (O^{18}) were evaluated in small forested catchments.

A great attention was paid to the soil as a key compartment of the hydrological cycle. Theoretical mathematical analysis of the Richards' equation and laboratory experiments reached conclusive evidence that the fingering effect of the soil water movement is impossible to describe using the standard theory of fluid transport in a porous material, which is based on a diffusion analogy (Richards' flow). New important findings describing the fingering as one of the manifestation of gravitationally destabilized flow were achieved. An original method for quantifying entropy production by fluid transport in a porous material was developed. Using

this method it was found that the entropy production by fluid transport is higher in the case of gravitationally destabilized flow than in the case of Richards' flow. A sudden oscillating discharge of water from porous material known as fill and spill effect was theoretically proved. This phenomenon of gravitationally destabilized flow of water into the watercourse causes flash floods on a scale of a smaller and middle basin. The original early warning system for flash floods was developed taking into account, besides the intensive precipitation, the potential formation of gravitationally destabilized outflow from the soil. This system representing the original output of the scientific research has been tested in the pilot headwater basin.