Description of the main research directions investigated by the institute

The Institute of Hydrodynamics includes two research teams focused on the physical and chemical properties of fluids with the special attention paid to water. The first team is directed to water related issues covering the problems both quantitatively and qualitatively. The second team solves the problems of physical characterisation of fluid flows ranging from nano- to reactor scales.

The Department of Water Resources is orientated towards the problems related to the drinking water treatment process, presence of micropollutants in raw water, estimation of soil water retention which is closely linked to ecohydrological monitoring. The following topics are covered by the team:

a) Algal organic matter removal;
b) Occurrence of microplastics and micropollutants;
c) Flocs/aggregates formation by coagulation-flocculation process;
d) Retention of water in the soil profile in changing natural conditions;
e) Precipitation data from climate models;
f) Ecohydrological monitoring.

Practical applicability of the results:

- Evaluation of the drinking water treatment process
- Optimisation of coagulation/flocculation processes in drinking water treatment
- Technological designs for water treatment plants
- Flood/Drought forecasting systems
- Water management in landscape protected areas

a) Algal organic matter removal

Algal organic matter (AOM) is a varied group of organic compounds produced by phytoplankton. Currently, AOM is commonly present in surface water bodies that serve as drinking water resources, and it often comprises majority of total natural organic matter in water. Increasing occurrence of AOM is associated to environmental factors such as elevated temperature and enhanced nutrient (especially nitrogen and phosphorus) supply, since these conditions favour the proliferation of phytoplankton and subsequently the AOM formation.

The removal of AOM during drinking water treatment is required for multiple reasons. It may comprise harmful toxins or taste and odour compounds, serves as a precursor for the formation of hazardous disinfection by-products, etc. However, its removal is complicated owing to the variable character of AOM, and distinct AOM fractions are particularly difficult to remove by conventional drinking water treatment technologies.

Different techniques aimed at AOM removal are investigated at the Institute. A necessary common prerequisite is AOM isolation and its characterization in terms of chemical composition, molecular weight distribution, charge, etc.

A critical step of surface water treatment is usually coagulation-flocculation, thus, a part of the research is devoted to increasing its efficiency for AOM removal and to elucidation of the involved mechanisms. The results imply that thorough optimization of coagulation conditions (particularly coagulant type and dose and coagulation pH value) is required to achieve maximum AOM removal, while the optimum is not uniform for different AOM fractions (e.g., AOM peptides/proteins and non-proteinaceous fraction). Thus, these fractions are studied also separately to enable in-depth insight into the reaction mechanisms. Additionally, since AOM is commonly present in water

together with other impurities, attention is paid to the mutual interactions of different compounds representative for surface water composition with AOM and its distinct fractions, and to the impact of the interactions on coagulation-flocculation. Focus is laid also on identifying such AOM components that may act as significant obstacles for coagulation (an example is complex forming peptides/proteins) and on the means of eliminating the associated adverse impacts.

A possible way of enhancing coagulation is pre-oxidation, which also has a potential to destroy some harmful AOM components such as cyanobacterial toxins. However, pre-oxidation may be detrimental to coagulation (particularly in case of organic compounds) when e.g. an inappropriate oxidant or its unsuitable dosage is applied. Thus, one research direction is to describe the impact of different modes of pre-oxidation on the coagulation-flocculation of AOM. A partial aim is to find optimum pre-oxidation conditions that enhance the removal efficiency of AOM, but emphasis is laid also on describing potential drawbacks of pre-oxidation and on identifying pre-oxidation modes that should be avoided for a particular type of AOM. Besides focus on the compound's removal, we also search for potential undesirable oxidation by-products. In addition, placement of the oxidation step elsewhere than prior to coagulation is also investigated.

Further, since certain fractions of AOM appear reluctant to either coagulation-flocculation or oxidation, also adsorption technology is investigated in this regard. An advantageous adsorbent utilized in drinking water treatment is granular activated carbon (GAC); therefore, adsorption of AOM constituents onto GAC deserves attention. We focus on the relationships between AOM, GAC, and influent solution properties, and also on the competitive adsorption between AOM and other water pollutants.

Thus, the removal of AOM, which is an ongoing challenge for drinking water treatment plants worldwide, is investigated at the Institute from different perspectives, while the research results bring useful information applicable to improve treatment efficiency and subsequently the quality of drinking water.

b) Occurrence of microplastics and micropollutants

Microplastics (MPs; plastic debris not exceeding 5 μm in size) are emerging contaminants of water environment. They occur in seawater, freshwater, and according to the recent investigation, also in drinking water, both from public supply and in bottled water. The ecological and toxicological impacts of MPs are still largely unknown; however, MPs raise concerns for many reasons. Besides possible physical effects associated to particle ingestion, attention is paid also to the content of residual monomers or additives in MPs, and to their ability to adsorb and carry hazardous chemicals.

One branch of the research at the Institute is devoted to MPs, particularly to their quantification and characterisation (in terms of size, shape, and material composition, etc.) in various aquatic samples, and also to MPs removal by water treatment technologies.

Quantification and characterization of MPs is performed especially for water collected at drinking water treatment plants (DWTPs). The fate of MPs at DWTPs working under ordinary conditions is very little explored, while they pose a promising barrier for MPs to enter drinking water. However, attention is paid also to potential MPs enrichment during the treatment processes, which might occur owing to the utilization of plastic materials. MPs down to the size of 1 μm are being determined at the Institute, which is currently very rare among the studies dealing with MPs. Analysis of only larger

MPs apparently leads to a significant underestimation of the results. Knowledge of MPs content in treated drinking water is important with regard to assessing exposure to MPs via drinking water, and quantification/characterisation of MPs in raw water and in water after distinct technological steps in DWTPs is necessary to evaluate the efficiency of common treatment technologies. These observations are also an important prerequisite for preparing relevant MPs samples utilized in future laboratory experiments aimed at investigating MPs removal. Current results imply that coagulation-flocculation and/or filtration may be effective for at least partial MPs removal, so these are to be investigated in detail.

Nevertheless, MPs are only one group out of the many anthropogenic pollutants, the occurrence of which in water requires attention. Research at the Institute focuses also on the determination and removal of other compounds such as pesticides and per- and poly-fluorinated organic compounds, or persistent organic pollutants in general. Since these are -in principle- not removable by coagulation-flocculation, rather the adsorption onto granular activated carbon or utilization of novelty adsorbents are considered as a promising solution for elimination of these undesirable micropollutants.

c) Flocs/aggregates formation by coagulation-flocculation process

Effective coagulation-flocculation process results in the formation of flocs/aggregates, in which the impurities to be removed are incorporated. At DWPTS, coagulation-flocculation is therefore followed by separation steps such as sedimentation, flotation, and/or filtration. The efficiency of aggregate separation is determined by the properties of the aggregates, and this is one of the research directions dealt with at the Institute.

Special attention is paid to characterizing aggregates resulting from coagulation-flocculation of AOM-containing water. Aggregate parameters such as size, shape, density or strength are determined by means of non-destructive optical analysis. The relationships between the factors that affect the key aggregate properties, such as AOM composition and character, coagulant type and dose, and hydrodynamic mixing conditions are investigated.

Optimizing the variable parameters with respect to AOM or other pollutant properties and to the required separation technique is a nuisance to assure efficient aggregate removal and to avoid difficulties such as undesirable aggregate breakage or worsened operation of separation facilities.

d) Retention of water in the soil profile in changing natural conditions

The hydrological cycle and water management represent the domain seriously endangered by the human activities and climate change. Soil water is a fundamental factor controlling partition of precipitation between runoff and evapotranspiration. The correct estimation of the amount of water stored in the soil is a prerequisite for the flood/drought forecasting systems, efficient agricultural and water management. The description of its spatial values relies mostly on the hydrological modelling approach, which requires the information about precipitation, evapotranspiration and soil properties.

The existing hydrological research of the Institute is therefore directed to the correct representation of evapotranspiration rate and incorporation of the temporally variable soil hydraulic properties in the modelling practice. The main purpose is to estimate efficiently the annual course of soil water content and to enable reliable long-term simulations without the necessity of data assimilation. This is lined with the recent change of modelling paradigm pursuing the notion that hydrological models should be less rigid and offer more flexible options for the parameter and model structure

utilization. The special attention is paid to: (1) an estimation of evapotranspiration in the forested environments, (2) an investigation of influence of temporally variable soil hydraulic properties on model efficiency in terms of soil water storage prediction, and (3) spatial variability of soil moisture content under different vegetation cover.

More specifically, the evapotranspiration flux from the different type of vegetation cover (beech and spruce forest, grassland, peat bog) is studied by means of field measurements of transpiration flux, interception of canopy and soil surface evaporation. The main aim is to quantify and correctly represent the seasonal evapotranspiration flux by the models so that the evapotranspiration loss may be studied on the long-term basis even for places or periods where the measurements were not available. Temporal variability of soil hydraulic properties is measured either in-situ or inferred from the inverse modelling tasks using different modelling approaches in different natural conditions (soil type, vegetation cover). The primary aim is to incorporate the temporal changes in soil structure in the modelling practice. The currently used generation of hydrological models does not include this phenomenon; albeit, it has already been reported in several studies. As the soil water regime is influenced both by vegetation cover and soil hydraulic properties the influence of both factors is studied on the long-term basis enabling the quantification of the climate change influence on the soil water retention. This is based on the unique long-term soil moisture records used as the basis for modelling the water balance of experimental sites.

e) Precipitation data from climate models

A climate change represents one of the most challenging topics of the current science. The global and regional climate models are established as a main data source for research of a potential climate change impact. Nevertheless, data provided by the climate models suffer from systematic errors caused primarily by a low spatial resolution and related simplification of important physical processes. As a consequence, an applicability of the data is limited and the raw climate model outputs cannot be directly used as an input for impact studies. From this point of view the precipitation is the most affected variable. Therefore, some form of post-processing (bias correction) is necessary prior to the data usage. Several bias correction methods have been developed to overcome the gap between the capability of climate models and the requirements of the impact modellers community. The methods are based on a simple or complex transformation of the original model data in order to match the statistical properties of the observed data. An application of bias correction represents the only way to assess the climate change impact in smaller scales and for this reason the bias correction is established as a standard procedure in the impact modelling.

Nevertheless, some serious concerns about the usage of bias correction have been currently presented, including the violation of physical consistency, the alteration of climate change signal and the non-consideration of the dependence between corrected variables. The research at the Institute is therefore oriented to these problems. Specifically, a new method of bias correction considering the cross-correlations between corrected variables was developed and the temporal stability of correlations in climate model data were investigated, including the robustness of correlation estimates. Nevertheless, some uncertainty regarding the bias corrections still persists and further research is needed.

f) Ecohydrological monitoring

Ecohydrological monitoring serves as a basis for the description of the hydrological and geochemical processes occurring in the environment. The measured data are

used for the modelling experiments and for a profound understanding of the changes of natural processes caused by climate change or human activities.

The insufficient length of existing observation data sets is often reported (they exhibit inhomogeneity, suffer from insufficient spatio-temporal resolution, and are 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. One of the research directions is therefore represented by the long-term monitoring of specific water fluxes in the landscape with the primary focus on the mountainous catchments. 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 monitoring is primarily aimed at fluxes of water, solutes and pollutants in different pools of the hydrological system encompassing precipitation, fog, throughfall, soil water, groundwater and stream water.

The Department of Fluid Mechanics focussed its research on the following topics:

a) Constitutive modelling of behaviour of non-Newtonian fluids;
b) Correlation between rheological characterization of polymer solutions and the resulting electrospun nanofibrous mats;
c) Identifying conditions of flow of compressible and incompressible fluids in nanoscale structures;
d) Development of advanced theoretical methods for flow-field analysis;
e) Hydrodynamic interactions in particle-laden flows and mixing reactors (both in terms of experimental and numerical approaches).

Practical applicability of the results:

- Completion of fluid flow description for simulation of individual polymer processes;
- Optimization of nanofibrous mats for specific purposes;
- Novel electro membranes, multifunctional fluid and vapour flow sensing structures;
- slurry pump design, hydrotransport of solid particles, waste disposal.

a) Constitutive modelling of behaviour of non-Newtonian fluids

Balance equations express the motion of fluid substances. To complete this set of equations it is necessary to introduce so called constitutive equation describing behaviour of the studied materials. Its proposal depends both on material composition and on the field in which the studied material is present (normal atmospheric, electric, magnetic, etc.).

According to a composition the materials (in our case fluids) are divided to two main groups – Newtonian and non-Newtonian. In the case of Newtonian fluids their resistance against flow (viscosity) depends only on temperature and pressure. The situation for the non-Newtonian fluids is much more complicated. Apart from the two above mentioned factors the viscosity subject to various input such as e.g. rate of deformation or stress. In other words, the relationship between stress and deformation

is nonlinear and therefore, the function (viscosity) relating stress and rate of deformation is rather complicated.

The Institute developed the constitutive modelling in three directions:

1) Rheological characterization of flow behaviour of polymer melts

Molecular-based differential models always exhibit two linear parameters. A number of nonlinear parameters oscillate between one and four in dependence on the used model. However, the models with only one nonlinear parameter (as e.g. the Giesekus one) suffer from impropriate description of some rheological characteristics. The general problem is that the macromolecules forming polymer melts are not identical (polydispersity index = 1) but there is a necessity to sort them in more groups with similar morphology. It reflects in an increasing number of modes n and hence, in increasing number (n x (1- 4) tuples) of nonlinear parameters causing their possible ambiguity and mutual physical misinterpretation. A relatively simple differential model with only one nonlinear parameter modifying the classical eXtended Pom-Pom (XPP) model was proposed and it was shown the same efficiency as in the case of often used XPP, PTT, PTT-XPP, and Leonov models. This was proved both in a linear viscoelastic region and in the case of Large Amplitude Oscillatory Shear (LAOS) measurements.

2) Master curves describing flow behaviour of feedstocks in the process of Powder Injection Moulding (PIM)

A description of feedstock (polymeric binder + metal or ceramic nano- and micro-particles) flow is problematic due to lack of the viscosity models respecting simultaneously powder filling and additive contents. The master curves describing feedstock flow behaviour were proposed approximating experimental data with a deviation within the experimental errors. These master curves respect both powder filling and additive contents and exhibit no adjustable parameters.

3) Empirical constitutive modelling of cosmetics products

The market of cosmetic products is very large and the consumers find the sensory attributes as the crucial ones. Evaluation of these attributes is financially expensive and time-consuming. There were proposed the empirical models describing rheological behaviour of the cosmetic products in such a way that the selected individual adjustable parameters can successfully substitute the sensory attributes.

b) Correlation between rheological characterization of polymer solutions and the resulting electrospun nanofibrous mats

Electrospinning represents one out of several processes of how to prepare nanofibrous mats that can be applied in various spheres such as tissue engineering, drug delivery, energy, the environments (air and liquid filtration, acoustic insulation), security (chemical and biological protection, bulletproof vests), to name a few. Originally this process came to an existence already in the 30s of the last century and was intensively developed during the World War II in connection with filters used in the gas masks.

Electrospinning is a technique at which an electric field is generated between a tip and a grounded collector by a high-voltage power supply. The drop of the polymer solution is stored on the tip, from which, in the presence of the electric field, a Taylor cone is created, and then a single viscoelastic fluid jet is ejected from the apex. As the charged jet travels in air, its diameter decreases due to simultaneous effects of the stretching of the jet at the high extension rates and the evaporation of the solvent.

The Institute concentrated to the following topics:

1) A way in which to prepare homogeneous solution prior to the process of electrospinning

Incomplete homogeneity results in nanofibrous mats of poor quality. Three ways of preparations consist of vibrational shaking, magnetic stirring and sonication, each exhibiting a stronger or a weaker impact on the homogenized materials. Vibrational shaking is rather considerate towards material morphology, however in some cases it is inefficient. In contrast, magnetic stirring - the only method characterised by invasive mixing - has a direct mechanical connection with the materials being mixed. Sonication can represent a more violent mixing dependent on circumstances. Unfortunately, in the majority of contributions on electrospinning the method of preparation is not mentioned and a characterization of the resulting solution can extremely differ from the original one. This deviates the expected qualities of the resulting mats. To control a solution preparation, we used rheological measurements carried out in an electrocell housed in the rotational rheometer.

2) Hydrophobic and magnetic nanofibrous mats

Nanofibrous composite membranes were prepared using polyvinyl butyral solution containing hydrophobic silica nanoparticles. Various surface modifications of the silica nanoparticles have been used to improve the waterproofing capacity of the membrane. Specifically, investigation was made into the effects of the rheological properties of the solution, as well as on fibre diameter as exerted by the applied voltage and the tip-to-collector distance. According to water contact angle measurements, the nanofibrous membranes reinforced with the incorporated silica nanoparticles demonstrated superhydrophobic surface properties.

Ultrasound treatment represents a very effective technique for distributing magnetic nanoparticles within polymer solutions. Adverse effects caused by sonication over time on the given nanofibrous membrane (polymer degradation and appearance of defects) were evaluated by using rotational (magneto)rheometry, electron microscopy, and magnetometry.

c) Identification of flow conditions of compressible and incompressible fluids in nanoscale structures

Nanoscale hydrodynamics deals with the motion of fluids in flow structures the dimensions of which are closely comparable with the size of the respective fluid molecules. The flow in such environments is determined primarily by interactions between the fluid and the structure surface molecules. These mutual interactions are of the principal importance in development of so called nanofluidics composed of channels the surface of which can selectively react with a penetrating both compressible and incompressible fluids. Moreover, electrically charged or chemically adjusted surfaces can control flow rates through channels or molecule adhesion to channel surfaces i.e., the principal phenomena, which are integral to flows in nanopore membranes or sensing structures of chemical and/or biological molecules. Accordingly, the Institute directed a research activity in the field of nanoscale hydrodynamics specially on interaction phenomena and their exploitable consequences.

1) Electrically–controlled permeation of vapours (compressible fluids) through carbon nanotube network–based membranes

DC voltage was used to identify the principles of penetration rate of chemical vapours through a conductive membrane composed of a layer of multiwalled carbon nanotube strengthened by a porous polyurethane non-woven mat. The penetration rate was affected by the vapour polarity and interaction of vapours and charged

nanotube surface. This interaction offers a wide range of combinations for the electric control of trans-membrane penetration by chemical vapours from the point of view a vapour compound separation, vapour withdrawal or a membrane gating.

2) Flow of resin through a carbon nanotube network as a sensing arrangement to detect a resin penetration through reinforcing textiles

The first time the resin flow was monitored by a carbon nanotube network embedded into a reinforcing textile in the casting form. The reason was to collect data on the resin penetration through the textile, to identify front flow advance, its branching, void formation as well as observation of final curing process. The collected data are applicable in numerical modelling of flows in complex casting forms with reinforcing textiles. Besides that, the suggested fluid flow measurement technique is the original one and may be used to improve understanding of flows in many various applications, generally.

3) The effect of adsorb molecules onto the carbon nanotube network surfaces on the electric conductivity and thermoelectricity of the network

Adsorption of oxygen molecules on carbon nanotube networks was analysed by means of Fourier transform infrared spectroscopy and X-ray photoelectron spectroscopy. The formation of new oxygen-containing functional groups on the surface of carbon nanotubes enhanced electrical conductivity of the network. Consequently, the network can realize direct energy conversion between heat and electricity and was examined as a self-powered thermoelectric device detecting adsorption of molecules.

d) Development of advanced theoretical methods for flow-field analysis

Rapid advances in computer science, numerical methods, and experimental techniques in fluid mechanics need to be followed both by a systematic study aiming at both the qualitative description of three-dimensional (3D) flow-fields and the theory of underlying equations of motion, the Navier-Stokes (N-S) equations. Firstly, flow modelling and numerical simulation of turbulent and transitional flows still lack a generally acceptable vortex-identification method. There is no universal criterion though the understanding of vortex dynamics (i.e. generation, evolution, interaction, and decay of vortical structures) should be based on objective and unambiguous detection schemes. Secondly, the mathematical theory of the N-S equations is concentrated on the study of qualitative properties of the solutions to the N-S equations. The Institute solved the following problems:

1) Advanced vortex identification

The original Q-criterion defines incompressible vortices as the regions in which the vorticity magnitude prevails over the strain-rate magnitude. One proposed modification takes into account compressibility by using the principal strain-rate difference vector. In the unified framework based on different approaches to averaging of the cross-sectional balance between vorticity and strain rate in 3D, new relations among the existing modifications have been derived. In addition, a new method based on spherical averaging is applicable to compressible flows, and it inherits a duality property which allows its use for identifying high strain-rate zones together with vortices. In comparison with the previous vortex-identification schemes, the new methods produce less noisy outcome (i.e. less contaminated by shear). Further, the earlier concept of the average co-rotation of infinitesimal radial line segments near a point has been extended to the case of contra-rotation. The tensor of contra-rotation has been introduced. It can be, similarly as the vector of co-rotation, further averaged

over “all planar cross sections” going through the examined point. Both the average contra-rotation and co-rotation, representing shear-free quantities, have been applied to vortical flow examples. Finally, a comparison of the stretching response for several popular vortex-dentification criteria and the recently proposed vortex vector (Rortex) was presented. The stretching sensitivity of the examined schemes significantly differs and, consequently, reopens the persisting vortex-identification problem that the requirement of orbital compactness of the motion inside a vortex contradicts with the allowance for an arbitrary axial strain.

2) Regularity and uniqueness of solutions to the Navier-Stokes equations

The fundamental questions concerning the regularity and uniqueness of solutions to the N-S equations remain open. The research focussed on the conditional regularity: the solutions are endowed with some additional properties and the regularity is then proved. The conditions on the vorticity, the velocity components and various combinations of entries of the velocity gradient or Hessian tensor have been imposed. To overcome the key problem, i.e. the estimate of the nonlinear convective term, the Troisi inequality has been used. Several generalized versions of the Troisi inequality both for the isotropic and anisotropic spaces were derived. For the case of the vorticity the Biot-Savart law was used. The criteria in the frame of the Lebesgue and Besov spaces were studied. In the case of the Besov spaces, a suitable form of the Bony decomposition was used giving an insight into the mutual interactions of the low, middle and high frequencies of the flow. As a result several new regularity criteria both optimal and non-optimal were received. The methods developed for the N-S equations were further applied to the incompressible magnetohydrodynamic equations, where the study of the mutual interplay between the magnetic field and the fluid velocity and pressure is the crucial part of the research. The regularity of the solution was proved under the condition that the gradient of the vertical velocity component and the horizontal magnetic field satisfy certain integrability conditions.

e) Hydrodynamic interactions in particle-laden flows and mixing reactors (both in terms of experimental and numerical approaches).

A description of hydrodynamic interactions in two-phase suspension flow is based on internal structure of the particle-laden suspension. These interactions can result in flow stratification and other phenomena affecting dissipation of flow energy (pressure drop) and mobility of transported particles (deposition-limit velocity).

The Institute carried out research in the following four directions:

1) Experimental investigation of the effect of pipe inclination on heterogeneous particle-laden flow

An influence of flow stratification for a given pipe inclination on experimentally observed variation in deposition-limit velocity and in pressure drops (manometric and frictional pressure drops) was determined. An experimental method evaluating the deposition limit velocity was proposed using gamma-ray measurements of variation of local solids concentration at the bottom of a pipe. Further, an anomalous pressure drop was identified in mildly descending pipes transporting partially stratified heterogeneous particle-laden mixtures. Its mechanism was described and explained using measured distributions of solids.

2) Macroscopic (layer-based) modelling of the effect of pipe inclination on heterogeneous particle-laden flow

A new layered model respecting pipe inclination was proposed for inclined flows (both ascending and descending) predicting various pressure drops, deposition-limit

velocity and simplified distributions of velocity and solids concentration. The Wilson-Tse nomogram widely-used for an evaluation of the deposition-limit velocity in inclined flows was generalised. Model efficiency was proved in determining anomalous pressure drop of the partially stratified flow in a descending pipe.

3) Microscopic modelling of fully-suspended particle-laden flow

The Two-Fluid Model (TFM) was applied to simulation of horizontal flow of non-stratified fully-suspended mixture in a pipe including detailed distributions of concentration, velocity and pressure drop. Based on model simulation results, optimised practical guidelines and consistency checks were proposed to improve an accuracy of the estimates and increase reliability of the solution. Finally, pipe size-up scaling tests and a specification of the applicability conditions justified usage of the TFM for flows at the pipes of industrial scales.

4) Flow field description in mixing tanks with radial impellers

The time-resolved PIV technique and LDA method were applied for a description of the unsteady velocity fields close to the impeller blades. The experimental data were used for verification of the numerical simulations (using DES and LES turbulent models) as well as semi-analytical approach, which was based on the conventional turbulent jet theory and the general theoretical framework of scalar dispersion.

Research activity and characterisation of the main scientific results

The main research activity of the Team in the evaluated period was focused on several topics corresponding to the main research trends of the Team. On the long-term basis, the Team is focused on optimisation water treatment processes, algal organic matter removal and quantification of water fluxes at various scales based on field observations and modelling.

The research topics in the field of drinking water treatment involved (i) removal of cyanobacteria, algae, and especially algal organic matter by various techniques and also in the presence of other impurities; (ii) characterisation and removal of micropollutants, such as microplastics; (iii) description of the formation and properties of aggregates formed during coagulation-flocculation in relation to their separation by sedimentation, flotation, and/or filtration.

In general, the research activities aim to develop water treatment technologies that will enable the production of high-quality drinking water from problematic water resources. The research itself is based on the description of the engaged principles and mechanisms.

In the field of hydrology, the main effort was put into the description of water retention in the soil profile. The temporal variation of the soil hydraulic properties was investigated namely from the perspective of its influence on the modelling practice and for the sake of hydrological forecasts. Apart from that the research was also conducted in the field of climate modelling, where the post-processing methods related to precipitation data from climate models were developed. These methods are crucial for hydrological climate change impact studies. Finally, the fluxes of water, its chemical composition and presence of various solutes were observed in a small experimental catchment in order to characterize the changes in natural processes caused both by human activity or climate change.

The most significant results from the evaluated period will be therefore presented in the parts corresponding thematically to the main research activities.

Algal organic matter removal

The occurrence of algal organic matter (AOM), a mixture of organic compounds produced by cyanobacteria and algae, is an ongoing challenge for drinking water treatment plants (DWTPs). AOM appears more frequently and/or its concentrations grow more intensively at many locations worldwide due to climate changes and anthropogenic impacts such as enhanced nutrient input to water bodies. AOM is highly undesirable in water since it might comprise harmful toxins or taste and odour compounds, serves as a precursor for disinfection by-products (DBPs) formation or as a source of assimilable carbon in the water distribution system, etc. Nevertheless, the removal of AOM is complicated owing to its highly variable character. An important step of surface water treatment is coagulation-flocculation (ID 447016). Our results when dealing with AOM of different species (*Microcystis aeruginosa*, *Merismopedia tenuissima, Chlorella vulgaris*) revealed that coagulation behaviour and subsequently removal efficiency greatly differs for AOM peptides-proteins and the non-proteinaceous fraction of AOM (ID 4446391, 474945, 494454). We determined the coagulation optima (the conditions under which maximal removal is already attained) for each of these AOM fractions when using different coagulants; the most important variables were coagulation pH and the coagulant dosage (ID 502798). The coagulation mechanisms were described in relation to the specific character of the AOM fractions, such as molecular weight (MW) distribution or charge properties associated with the content of

ionisable functional groups in AOM. The research results were utilized when optimizing technologies for DWTPs that had problems to handle the intensive occurrence of AOM in their raw water. We cooperated even with the largest Czech DWPT Želivka (max. output 7,000 L/s), water source which is significantly affected by an increase in AOM content (ID 501634).

Besides AOM alone, we deal also with the removal of AOM in the presence of other raw water components. Naturally, AOM commonly appears in water together with algal/cyanobacterial cells. The phenomenon was investigated for cyanobacteria *M. tenuissima* (ID 474945). This species is of great interest due to its wide ecological niche, small cell size, and appearance throughout in the entire water column. Under the optimized coagulation conditions, we attained very high (up to 99 %) cell removal either when coagulating the cells alone or in the presence of *M. tenuissima* AOM (specifically cellular organic matter – COM). However, COM altered the coagulation optimum for cell removal – it changed the effective coagulation pH range and interestingly, lowered the necessary dose of coagulant. Thus, the interactions between the cells and COM released from them must not be overlooked. Another approach for separating cells is alkaline flocculation, currently rather utilized for algae harvesting. This principle was studied on *C. vulgaris*, with an emphasis put on describing the effects of variables such as pH, ionic strength, and concentration of calcium and phosphate ions; the conditions resulting in efficient flocculation were defined (ID 487866).

Further, despite AOM often comprises a majority of natural organic matter (NOM) present in surface water bodies, it is also commonly accompanied by other kinds of NOM, of which humic substances (HS) are the most important. Thus, the simultaneous removal of AOM (specifically COM peptides-proteins of *M. aeruginosa*) and HS and their mutual interactions were studied (ID 446391). It was shown that under optimized coagulation conditions, COM may improve the removability of HS. To better describe COM protein-HS interactions, a model protein (BSA – bovine serum albumin) was employed in the experiments and appeared to be a good model compound representing a sort of AOM proteins.

Despite a significant proportion of AOM is removable by coagulation and AOM may also contribute to the removal of other substances under specific coagulation conditions, some AOM residuals tend to remain in water after coagulation. Pre-oxidation conducted prior to coagulation represent a possible technique for improving removal efficiency, and it is also a part of our research (ID 471168). Very good results were obtained for permanganate pre-oxidation and subsequent coagulation of *M. aeruginosa* COM peptides-proteins. Up to 90% removal of the peptides-proteins was reached, while contained microcystins were efficiently eliminated owing to the involvement of the pre-oxidation step. Moreover, pre-oxidation apparently prevented the formation of dissolved metal-protein complexes that otherwise interfered with coagulation under certain pH values. This method for improving AOM removal by means of gentle permanganate pre-oxidation was patented (ID 453894) and already successfully utilized at some DWTPs.

The residual AOM after coagulation or even after pre-oxidation-coagulation is typically formed by its low-MW fraction. This is especially the case of non-proteinaceous AOM, which usually contains a significant proportion of low-MW components. However, presence of low-MW peptides or their constituents (amino acids) is also problematic. Such compounds are not removable by coagulation and further treatment is required. We investigated the applicability of adsorption onto granular activated carbon (GAC) for the purpose of removing low-MW AOM, i.e., model

amino acids that are commonly comprised in AOM were utilized (ID 463137). GACs of different physicochemical properties were investigated, and also the effects of factors such as adsorbate initial concentration, solution pH and ionic strength were studied. Consequently, relationships between the variables were proposed and the distinct adsorption mechanisms were identified. Understanding of the adsorption process is essential for its effective utilization in practice, and our findings were applied in designing adsorption technology for removing residual AOM e.g. at the DWTPs in Kutná Hora (max. output 150 L/s) and Světlá nad Sázavou (max. output 30 L/s) (ID 520983).

To conclude, we performed a complex research aimed at the efficient removal of AOM (ID 497263). Various technologies involving coagulation-flocculation, oxidation, or adsorption were studied (ID 446391). Additionally, we dealt also with the interactions of AOM with algal/cyanobacterial cells and other common raw water constituents, including remaining NOM fractions. Attention was then paid to the impacts on water treatment processes. Focus was also laid on the removal of the most problematic AOM fractions, such as cyanobacterial toxins or other low-MW components (ID 471168, 474945). Investigation of AOM removal during drinking water treatment is of a broad international interest, and our results are not only of a scientific value, but some are clearly applicable in water treatment practice. With regard to the high demand for quality of drinking water and its limited resources most often containing a range of undesirable compounds, inventing and improving water treatment technologies is a necessity. We believe that our research significantly contributes to international knowledge in this field. Also, cooperation with the University of New South Wales (Australia) and Cranfield University (UK) on this topic has been established (ID 447016, 471168, 497268, 506527).

Microplastics

A very current topic is the occurrence of microplastics (MPs) in aquatic environments. MPs are defined as plastic debris not exceeding 5 mm in diameter; they greatly differ in their shape, size and may encompass a wide range of materials. So far, investigations prevailingly dealt with MPs in oceans and seas, and to a very limited extent in freshwaters.

We performed the very first study that determined MPs down to the size of 1 μm in raw and treated drinking water (ID 492128). This investigation was conducted at three DWTPs (supplied by surface water) that employ different treatment technologies. This way we also provided a unique preliminary insight into the removal of MPs at DWTPs. The numbers in treated water exhibited around 70-80% lower participation of MPs than in raw water before the treatment. Additionally, characterization of MPs in terms of their size, shape and material was also carried out, both for raw and treated drinking water samples. We were, therefore, able to identify the individual types of MPs that tend to remain in drinking water after conventional treatment. The most problematic ones from this point of view are the smallest MPs within the size range of 1–10 μm. They represented an overwhelming majority – especially in treated water, despite the fact that they were neglected in most previous studies owing to the difficulties in their sampling and measurement. Moreover, some plausible relationships between the shape and removability of MPs were also suggested based on the results of our study. We also found the prevailing materials comprising MPs at the DWTPs. Applying knowledge with MP analysis from this research, we also conducted a determination of MPs at some other DWTPs that showed their interest. Again, the contribution of MPs

< 10 μm proved to be the most significant, despite great differences in MP numbers per water volume were observed in dependence on the water sources.

It is of note that potential toxicological effects of MPs are still largely unknown, despite many investigations have been done on different (especially aquatic) organisms. Some preliminary studies proved interaction of MPs with human cells, and concerns with regard to MPs stem also from their tendency to sorb hydrophobic organic pollutants. Nevertheless, considering the precautionary principle and the growing production of plastic materials, the fate of MPs at DWTPs is of a great interest since their technology can pose a barrier for MPs to enter drinking water. In order to precisely define the research needs regarding MPs removal by DWTP technologies, we elaborated and discussed MPs appearance in water resources, removability of MPs at wastewater treatment plants (that have received much greater attention so far than DWTPs), and (dis)similarities of MPs to common water pollutants (ID 502192). It enabled us to establish appropriate setup for an ongoing research of MP removal by distinct technologies.

In summary, we conducted the first investigation of MPs abundance and character in raw and treated drinking water originating from surface water bodies. We performed a study that covered MPs down to the size of 1 μm, which is very unique (ID 492128). The results provide valuable information on approximate MPs removal by conventional drinking water treatment, and we defined the types of MPs that appear the most problematic and therefore deserves the highest attention. These conclusions are not only useful for our further research but significantly contribute to the global knowledge in this field.

The obtained results of our research were also used in practice – in the scientific reports for several DWTPs - Káraný (max. output 2,000 L/s), Podolí (max. output 1,500 L/s), Plzeň (max. output 1,000 L/s), Milence (max. output 400 L/s), etc. For these DWTPs we determined MPs in raw and treated water and also established an efficiency of MPs removal by different water treatment technologies (ID 504505, 501632).

Flocs/aggregates formation by coagulation-flocculation process

Research is also focused on the formation of flocs/aggregates in the coagulation-flocculation process and their properties (such as size, shape, density or settling velocity), which are crucial for efficiency of their separation (ID 497268, 506527). It is known that each of the used separation technologies (sedimentation, flotation and sand filtration) needs the flocs with different properties. For separation by sand filtration, very small flocs (generally < 50–60 μm) with high density penetrating the entire volume of the filter bed are required. Sedimentation needs large homogeneous flocs (> 100 μm) with high density and thus with higher settling velocity resistant to the effects of tangential forces. For a dissolved air flotation (DAF), flocs of tens of μm (preferably 25–50 μm) with a low density close to the density of water are recommended.

Concerning that algae/cyanobacteria and their AOM comprise the substantial part of water-polluting substances, we aimed at the determination of the effects of AOM and cells of different cyanobacterial and algal species on the properties of flocs (ID 497268). We have published one of the few existing studies dealing with properties of flocs made of AOM. In this study a comparison of flocs containing kaolinite, COM-peptide/proteins of *Microcystis aeruginosa* and both components together coagulated with Al or Fe coagulants using a broad range of velocity gradients was made. We found that COM-peptide/proteins (due to their high MW) increased the floc size significantly

in comparison with flocs containing only kaolinite. Simultaneously, the effect of the coagulant used (Fe vs. Al coagulants) was proved to be very significant since Fe produced considerably larger flocs than Al. The finding fact that increasing velocity gradient *G* (shear rate) used for floc formation produces smaller and more compact flocs was confirmed also for AOM flocs. Moreover, the size-*G* dependence showed additional interactions that are not employed in kaolinite-only flocs. Further research examined the properties of flocs made of five algal/cyanobacterial species with different cell morphology, their AOM and Al coagulant (ID 506527). It was shown that floc properties are generated by the microorganism species and by the AOM composition rather than coagulation conditions (dose and pH value).

The obtained results were used in practice – in the scientific reports for technology optimization tailored to the needs of several DWTPs (Kutná Hora, Tlumačov, Světlá nad Sázavou, etc.) (ID 497211, 510696, 520983). For example, we made a recommendation for the Kutná Hora DWTP, where aluminium sulphate at pH = 7 (optimum pH for Al removal) was originally used for coagulation (ID 510696). Nevertheless, the optimum pH for organic matter removal proved to be much lower and the coagulation efficiency was not sufficient. We proposed replacing aluminium sulphate coagulant with ferric sulphate and adjusting pH to acidic value (around 5), where organic matter present in raw water was removed efficiently together with Fe. Moreover, replacing Al with Fe coagulant has led to the formation of larger flocs more suitable for separation in rectangular sedimentation tanks.

Concerning a non-uniform manner of water treatment control in the DWTPs and the technological problems following from this fact, we created a certified methodology of jar tests for water treatment optimization (ID 520983). We explained difficulties arising from the incorrect conducting the jar test procedure and provided detailed guidelines for pH and coagulant dose optimization including examples of jar test data recording, processing and evaluation. The jar test methodology was then distributed among the DWTP managers, engineers and lab workers (ID 518185).

As other practical outputs, a laboratory flocculation device (based on the Taylor-Couette reactor principle, ID 511416) with the possibility of floc properties characterization and a pilot plant of flocculation - ID 492234 (both registered as utility models) were developed. The pilot plant consisted of a mixing tank with two separated impellers allowing independent mixing intensities (Rushton turbine and 4-blade propeller), an agent dosing (pH adjusting agents, coagulants) and a rapid gravity sand filter with pressure transducers installed along a filter bed. It was installed in the Kutná Hora DWTP and serves for flocculation pilot tests. The results can be used directly for the DWTP operation/control. We are also the authors of water treatment technological designs for a number of the DWTPs (Světlá nad Sázavou, Kutná Hora, Cvekov, Hrobice, Jince, etc.).

Retention of water in the soil profile

The soil water retention represents one of the key research topics of the Team. The Team possesses experimental sites used for observation of the water fluxes in the soil profile that serve as a basis for the modelling experiments. The main aim is to characterise accurately the amount of water hold in the soil, which represents a necessary input for the hydrological forecasting systems or agricultural water management.

An attention was paid especially to the description and modelling of the temporally variable soil hydraulic properties (SHPs). The activity was triggered by the finding that the soil moisture simulation of the mesoscale Soil and Water Integrated Model (SWIM)

exhibited a good correspondence with the observed data in the warmer season (April–August) in a small-scale forested catchment (ID 443642). Both the dynamics and the magnitude were estimated sufficiently well. On the other hand, the colder season does not comply satisfactorily with the modelled data, as observed declines of moisture content (in the non-precipitation periods) had no model response. The temporal variation of the soil hydraulic properties could be one of the causal factors.

Therefore, we explored the long-term temporal variation of SHP (ID 476340) based on the ponded infiltration experiments performed annually in a grid of permanent measurement points (18 spatial and 14 temporal replicates). Single ring infiltrometers were installed in 2003 at a meadow site in the Bohemian Forest, Czech Republic. Significant changes of infiltration rates were observed after first four years. It was hypothesized that these changes can be attributed to structural changes of the soil profile possibly related to combined effect of biological activity, climatic conditions and experimental procedure. Interestingly, the temporal changes can partly be described as fluctuations between seemingly stable infiltration modes.

The spatio-temporal variability of the soil hydraulic properties was, on the intra-seasonal basis, also investigated in the uncultivated Fluvisol (ID 505401). Specifically, a small-scale experimental plot (10 × 10 m) was used during four field works evenly distributed in one vegetation season (8 months) in order to demonstrate the importance (representativeness) of sufficient sampling in time and space. The measured values of SHP were used for the HYDRUS-1D model in order to observe the influence of the spatial and temporal variability on the modelled soil water regime. In summary, the high spatial variability of soil hydraulic properties in the uncultivated Fluvisol (representing permeable sandy fluvial sediments) proved to be superior to their temporal changes and it is therefore worth quantifying its extent for modelling purposes. The described variability of SHP will serve as a benchmark for the further investigation of the soil organic matter (SOM) influence on the soil water regime in field conditions. The first step was done in the study (ID 499005) investigating the influence of biochar (pyrolized organic matter) application on two contrasting soils (sandy and clay soils). The effect of SOM on soil hydraulic properties (SHP) was studied and the interactions between water and the biochar surface were described. The added SOM caused intensive swelling, which decreased the bulk density and enhanced the water holding capacity (up to 5 % in the case of sandy loam and 5 % biochar dose), and significantly decreased *Ks* in both soils (with a maximum difference of 83 %).

As the above-mentioned studies reported the importance of not only temporal but also spatial variability of SHP the next work (ID 510658) was focused on the description of soil water dynamics at four sites with different land cover types, namely beech forest, conifer forest, meadow and clipped grass. The analysis was based on soil tensiometer measurements from five consecutive vegetation seasons (comprising both wet and dry years). The soil water balance was studied by the HYDRUS-1D model. The highest pressure heads were observed at the grassland site, followed by the meadow site and forested sites. The differences between the spruce forest (*Picea abies*) and beech forest (*Fagus sylvatica*) were evident namely in dry periods, when the beech site was experiencing lower pressure heads. The inspection of the soil water balance revealed different rates of evapotranspiration at all sites given namely by the water consumption efficiency and differences in interception rates, vertical distribution of the roots, and soil hydraulic properties.

Besides the measurements, the temporal variability of the SHP was used for a design of a new strategy concerning the soil water model calibration (ID 468168). First, the model parameters were allowed to vary between two distinct parts of the year

– dormant and vegetation seasons – and also from year to year in the calibration procedure. Consequently, two sets of average model parameters corresponding to the dormant and vegetation seasons were proposed. The overall Nash-Sutcliffe coefficient increased from 0.64 to 0.79 and from 0.55 to 0.80 concerning two utilized soil water bucket models. The variability of the warm and cold parameter sets between particular years was more pronounced in the warm periods.

The model calibration was also shown to be an important issue. Hence, we developed a novel methodology and software for the optimisation of a rainfall-runoff modelling (ID 480548) using a genetic algorithm (GA) with a newly prepared concept of a hydro random number generator (HRNG). The new HRNG generates random numbers based on hydrological information and it provides better numbers compared to pure software generators. The GA enhances the model calibration and the goal is to optimise the calibration of the model with a minimum of user interaction. The obtained results indicated that the HRNG provides a stable trend in the output quality of the model, despite various configurations of the GA.

The primary motivation for the research in the area of the soil water retention is represented by the importance of the initial hydrologic conditions (represented by the amount of water stored in the soil and snowpack) on the efficiency of the hydrological forecast. This was stressed in the study (ID 445334) concerning the probabilistic seasonal hydrological forecasts with a lead-time of one month. In this study, the LARS-WG weather generator was used to compensate for the meteorological datasets of insufficient length for the Ensemble Streamflow Prediction (ESP) system. The modified ESP approach proved to be more efficient in the majority of months compared both to the original ESP method and reference forecast (based on probability distribution of historical discharges). The improvement over traditional ESP was most obvious in the narrower forecast interval of the expected runoff volume.

The overall effort to establish an efficient hydrological forecasting system (ID 518126) (based on an accurate estimation of the soil water saturation of the area) resulted in a project in which one operating system was developed and put into practice covering the region of 100 km^2. Three devices used for the real-time monitoring of water levels and soil water content were developed within this project (robust monitoring unit – ID 457212, water level monitoring station – ID 457211 and soil water tensiometer – ID 457213). The operating system includes the instrumentation, software, dispatching and methodology of sophisticated local warning system against flash floods considering the latest knowledge about hydrodynamics mechanisms of the runoff formation. Each of dangerous factors and their combination are considered: (1) extreme rainfall usually after the long-term drought, (2) saturation of the soil, (3) water repellency of the soil, (4) gravitationally destabilized water flow in the soil.

Precipitation data from climate models

The climate change represents one of the most important and the most challenging topics of the recent science. Over the last decade the climate models have been established as a fundamental data source for the research of a potential climate change impact. Nevertheless, the outputs from climate models suffer from systematic errors introduced primarily by the low spatial resolution of models and by the related simplification of important physical processes. As a consequence, some form of statistical post-processing (bias correction) is necessary before the climate model outputs are applied as an input for climate change impact assessment studies. Precipitation represent a crucial input for most climate change studies and at the same time it belongs to meteorological variables that are most affected by bias. Therefore,

the effort was primarily focused on developing of methods improving an applicability and reliability of the climate model precipitation outputs. Specifically, two studies related to this topic were conducted.

The attention was paid to one of the most problematic points of the current bias correction approaches, which is the fact that the corrections are applied separately for an individual spatial point and meteorological variables (ID 462443). As a result, the correlation structure of corrected data preserves the bias introduced by the climate model, although the statistical indicators of the individual corrected variables show good agreement with observations. This can impair the modelling of many hydrological and biological processes, for example the runoff generation or crop yield. In the study the novel approach to bias correction was presented, which naturally corrects the correlation structures of multivariate data as well as the statistical indicators of individual variables. The introduced method consists in an orthogonal rotation of the data coupled with a linear rescaling of individual variables, the parameters of this process are derived from the principal component analysis. We also provided an explanation of the linear nature of commonly used correction methods, which enables to combine them with the newly introduced method and reach the highly accurate results. The most recent climate models (from the EURO-CORDEX project) have been used for the verification which proved the merits of the proposed method.

The applicability of the method presented above is conditioned by a certain stationarity of the correlation structures. Therefore, in the next step the temporal stability of the correlation structures of the climate model data was investigated (ID 502344). The changes of correlation structures of a multivariate precipitation model dataset (originating from the EURO-CORDEX experiment database) were assessed. In the first stage it was found that the changes of correlation coefficients were high in many cases, which indicated a considerable instability of the correlation structures. Nevertheless, in the second stage the statistical significance of the changes was tested using the bootstrap approach and it was found that most of high changes were statistically insignificant. Further analysis showed, that the instability was caused by outlying values. It was demonstrated that a few outliers can strongly affect correlation estimates even in large dataset. In turn, any statistical method dealing with sample correlation (including the bias correction procedures) can provide misleading results. Therefore, the exploratory procedure was proposed, making a distinction between ordinary outliers (i.e. values exceptionally small or large) and dependence outliers (values deviating from dependence structures). The procedure enables to explore an internal structure of large multivariate datasets and clearly indicate the presence and importance of dependence outliers. From another point of view, the removal of outliers showed that the correlation structures of precipitation data from climate models are quite stable in time. This indicates, that the climate projections of daily precipitation can be interpreted as a linear transformation of an initial state, which may have serious consequences and simplify the climate change impact studies.

Ecohydrological monitoring

Intensive hydro-ecological monitoring serves as a basis for the description of the hydrological and geochemical processes that occur in the environment. The datasets are then used for the modelling experiments (namely incorporating described significant processes into the modelling practice) and for a profound understanding of the changes of natural processes caused by climate change or human activities.

Several experimental sites were used for the monitoring of the contribution of deposited precipitation (DP) to the falling precipitation (FP) amount (ID 442051). An

automatic device for DP weight measurement was used. The results of deposited and falling precipitation measurements in three localities in the Czech Republic were summarized – Suchdol, Prague (capital of the Czech Republic), Poledník (Bohemian Forest), and Smědava (the Jizerské hory Mts.). Second and third introduced stations are situated in the mountainous parts of the Czech Republic. The daily averages of the DP totals equalled to 0.074 mm for Suchdol, 0.112 mm for Poledník, and 0.103 mm for Smědava stations. The overall ratios of DP to FP were found to be between 1 % and 3 %, which represents 27–41 mm per year. These amounts of water are not very important from the hydrological point of view, but they attain much higher importance due to the fact that significantly higher concentrations of pollutants are in DP compared to FP.

Further, the Team participated in studies concerning the fluxes of sulphur and nitrogen in the Czech Republic. First, the temporal development and spatial variability of sulphur (S) and inorganic nitrogen (N) concentrations in bulk precipitation and in throughfall was assessed (ID 460321). Overall significant declines of SO4 concentration in bulk and throughfall precipitation, as well as NO3 and NH4 concentration in bulk precipitation, were observed. Moreover, the new method for the prediction of S and N depositions based on emission rates was developed. Furthermore, changes in atmospheric deposition, stream water chemistry and solute fluxes in small forested catchments was investigated (ID 476536). These changes in atmospheric inputs have been associated with expected changes in levels of acidity, sulphate and base cations in streams. Soil retention of S appeared to partially explain rates of chemical recovery. In addition to these changes in acid–base chemistry we also observed unexpected changes in nitrogen (N) biogeochemistry and nutrient stoichiometry of stream water, including decreased stream N concentrations. The declines in phosphorus adsorption with increasing soil pH appear to contribute to the relationship between C, N, and P in our study catchments. Our observations suggest that catchment P availability and its alteration due to environmental changes (e.g. acidification) can have profound effects on N cycling and catchment N retention that have been largely unrecognized.

Besides the atmospheric deposition and stream water chemistry, the energy balance was thoroughly inspected (ID 500537). The reason was that longwave radiation, as part of the radiation balance, is one of the factors needed to estimate potential evapotranspiration (PET). Since the longwave radiation balance is rarely measured, various computational methods have been designed. The difference between the observed longwave radiation balance and modelling results were quantified using two main procedures outlined in FAO24 (relying on the measured sunshine duration) and FAO56 (based on the measured solar radiation) manuals. The performance of these equations was evaluated in the April–October period over eight consecutive years at the Liz experimental catchment in the Bohemian Forest. The coefficients of both methods, which describe the influence of cloudiness factor and atmospheric emissivity of the air, were calibrated. The Penman-Monteith method was used to calculate the PET. The use of default coefficient values resulted in the errors of 40–100 mm (FAO56) and 0–20 mm (FAO24) for the seasonal PET estimates (the PET was usually overestimated). Parameter calibration decreased the FAO56 error to less than 20 mm per season (FAO24 remained unaffected by the calibration). The FAO56 approach with calibrated coefficients proved to be more suitable for estimation of the longwave radiation balance.

Research activity and characterisation of the main scientific results

The Team of Fluid Mechanics focussed its research on the following topics:
a) Constitutive modelling of behaviour of non-Newtonian fluids;
b) Correlation between rheological characterization of polymer solutions and the resulting electrospun nanofibrous mats;
c) Identification of flow conditions of compressible and incompressible fluids in nanoscale structures;
d) Development of advanced theoretical methods for flow-field analysis;
e) Hydrodynamic interactions in particle-laden flows and mixing reactors (both in terms of experimental and numerical approaches).

In the following the main results obtained in the individual topics are introduced.

ad a) Constitutive modelling of behaviour of non-Newtonian fluids

The role of the Gordon–Schowalter derivative term in the constitutive models

Constitutive models that complete the set of equations describing the flow of polymer melts 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 proposed modified eXtended Pom-Pom (mXPP) model (just one non-linear parameter per mode) implementing the GS derivative term (one additional nonaffine motion parameter per mode) was improved (documented on LDPE, HDPE, and poly(vinyl butyral) materials), and a comparison with the often used exponential Phan-Tien–Tanner (PTT) and PTT-XPP models (a priori containing the GS derivative term) was very good.

Flexibility of differential constitutive models evaluated by large amplitude oscillatory shear (LAOS) and Fourier transform rheology

Using Fourier transform rheology, the Giesekus, exponential Phan-Tien and Tanner, and the proposed modified eXtended Pom-Pom constitutive models were examined in the non-linear regime represented by large amplitude oscillatory shear (LAOS) measurements. For the experiments a 5 wt.% solution of poly(ethylene oxide) (molecular weight 1000 kg/mol) solved in dimethyl sulfoxide was used. The minimal number of harmonics (15) required for an adequate reconstruction of the original raw time-stress signal was shown. An emphasis was paid to simultaneous consideration of the normalised stress magnitudes and phases of individual harmonics in the fitting procedure adjusting non-linear parameters of the studied constitutive models.

Two ways to examine differential constitutive equations: initiated on steady or initiated on unsteady (LAOS) shear characteristics

The exponential Phan-Tien and Tanner, Giesekus, Leonov, and modified eXtended Pom-Pom differential constitutive models were evaluated in two ways: with regard to steady shear characteristics and with regard to large amplitude oscillatory shear characteristics of a solution of poly(ethylene oxide) in dimethyl sulfoxide. Efficiency of the models with nonlinear parameters optimized with respect to steady shear measurements was evaluated by their ability to describe large amplitude oscillatory

shear (LAOS) characteristics. The reciprocal problem was also analysed: the nonlinear parameters were optimized with respect to the LAOS measurements, and the models were confronted with the steady shear characteristics. In this case - optimization was based on the LAOS measurements - equal emphasis was made to both real and imaginary parts of the stress amplitude. The results showed that the chosen models were not adequately able to fit the LAOS characteristics if the optimization of nonlinear parameters was based on steady shear measurements. It follows that optimization of nonlinear parameters is much more responsible if it is carried out with respect to the LAOS data.

Visualization of Elongation Measurements Using an SER Universal Testing Platform

For proper evaluating of the differential constitutive models it is necessary to acquire responsible experimental data for steady and transient elongational viscosity. A Sentmanat Extension Rheometer represents one out of a few experimental devices for the measurement of elongational viscosity of polymer melts and at present has a dominant role. However, the appropriateness of this technique for individual polymer materials is not sufficiently apparent and in some case is disregarded or ignored. The proposed visualization technique is 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 LDPE Escorene. Two various imprinted patterns were applied. First, the upper and lower contours were 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 was charted for evaluating possible inhomogeneity of the sample. A deviation from the theoretical (exponential) curves can serve as an indication according to which it is possible to categorize the materials with respect to possible evaluation of their elongational viscosity by means of the SER rheometer.

Master flow curves as a tool to modelling ceramic injection moulding

Compounds used for Ceramic Injection Molding (CIM) are rheologically complex materials. The applicability of currently available mathematical models to CIM systems fails due to high number of variables playing a significant role: binder composition, powder morphology and loading as well as concentration of processing aids. We derived the way to overcome this issue with a model, where a set of its parameters is a priori given regardless the contents of powder or additional ingredients in a feedstock. Then, the relative viscosity of an individual composition of a CIM feedstock was obtained only by inserting the corresponding concentrations of powder (aluminium oxide) and additive (stearic acid). The proposed master curve exhibited the fixed functional structure common for 36 composition combinations arising from Al_2O_3 powder loading (0-50 %) and stearic acid concentration (up to 5 %). The deviation from the measured values did not exceed an experimental error.

Relation between sensory analysis and rheology of body lotions

Evaluation of sensory attributes of cosmetic products is traditionally based on sensory panels. However, in some cases a suitable candidate method which can substantially reduce time and costs is the use of instrumental analysis that can detect

relatively very small changes of entry ingredients. It was shown that a description of chosen sensory attributes can be responsibly carried out by rheological measurements, i.e. through the attained numerical values of the parameters appearing in the proposed empirical models characterizing shear viscosity of body lotions.

ad b) Correlation between rheological characterization of polymer solutions and the resulting electrospun nanofibrous mats

Magnetorheological behaviour and electrospinning of poly(ethylene oxide) suspensions with magnetic nanoparticles

Behaviour of a novel magnetorheological (MR) fluid based on poly(ethylene oxide) aqueous suspensions was compared with that when 'classical' carrier fluids are used. This was carried out by detailed MR measurements and by the sedimentation tests. In our case, these tests are important only in their initial stages as they serve as an evaluation of homogeneity of the MR fluid with magneto-nanoparticles (MNPs) directly applied to an electrospinning process under no magnetic field. The resulting effect is a more uniform distribution of MNPs within nanofibrous webs, thus ensuring homogeneous magnetic properties of these resulting membranes. The preferred application of MR fluids exhibits the following advantages which have resulted from the development of this branch in the past few decades: excellent efficiency of the MNPs regarding their magnetic properties (application of nanofibrous mats in practice), sophisticated core-shell structures ensuring very good sedimentation stability (and consequently an even distribution of MNPs in the process of electrospinning as mentioned above) and resistance against mechanical disturbances caused by the presence of MNPs (tearing, cutting, scissoring) in electrospun mats due to the smooth surface of MNPs.

Nanofibrous web quality in dependence on the preparation of poly(ethylene oxide) aqueous solutions

The method of preparation of polymer solutions significantly influences the quality of the corresponding electrospun nanofibrous webs. However, this factor is often ignored, and in a majority of presentations concerning the electrospinning process, the applied method is not mentioned. There were compared the influence of magnetic stirring, vibrational shaking and ultrasonication on a solution of poly(ethylene oxide) in distilled water. Along with the methods of preparation, other parameters were altered such as concentration, intensity of mixing and molecular weight. The quality of nanofibrous webs was determined by scanning electron microscopy using digital image analysis (diameters of fibres, appearance of beads and other unwanted phenomena, etc.). The rheological measurements are in correspondence with the visualization conclusions. The best results from the viewpoint of electrospinning were achieved with moderate magnetic stirring.

Magnetorheological characterization and electrospinnability of ultrasound–treated polymer solutions containing magnetic nanoparticles

In this case ultrasound treatment represents a very effective and practically unique technique for distributing magnetic nanoparticles within polymer solutions. Adverse effects caused by sonication over time on the given nanofibrous membrane (polymer degradation and appearance of defects) were evaluated by using rotational magnetorheometry, electron microscopy and magnetometry. A magnetorheological approach was selected to estimate the optimal duration of sonication, and findings were experimentally verified. It was concluded that according to magnetorheological

efficiency, the sonication of a PEO solution containing MNPs is limited (under the pre-set conditions of sonication, i.e. intensity and frequency) for the preparation of a high quality magnetoactive membrane.

Superhydrophobic poly(vinyl butyral) nanofibrous membrane containing various silica nanoparticles

Nanofibrous composite membranes were prepared by the elecrospinning process of poly(vinyl butyral) solution that contained hydrophobic silica nanoparticles (SiO_2). Various surface modifications of the silica nanoparticles have been used to improve the waterproofing capacity of the membrane. Specifically, investigation was made into the effects of the rheological properties of the solution, as well as on fibre diameter as exerted by the applied voltage and the tip-to-collector distance. The different sizes of the silica nanoparticles among the electrospun nanofibres resulted in a hierarchical structure, which is critical for engendering superhydrophobic properties. According to water contact angle measurements, the given PVB nanofibrous membrane reinforced with the incorporated silica nanoparticles demonstrated superhydrophobic surface properties.

Characterization of poly(ethylene oxide) nanofibres - mutual relations between mean diameter of electrospun nanofibres and solution characteristics

The quality of electrospun poly(ethylene oxide) (PEO) nanofibrous mats subject to a variety of input parameters. In our study three parameters were chosen: molecular weight of PEO, PEO concentration (in distilled water) and shear viscosity of PEO solution. Two relations free of any adjustable parameters were derived. The first, describing the initial stage of an electrospinning process expressing shear viscosity by means of PEO molecular weight and concentration. The second, expressing mean nanofibre diameter by means of concentration and PEO molecular weight. The proposed relations were compared with the experiments and the mean deviations are practically within the experimental errors. Based on these simple mathematical relations, it is possible to control the mean nanofibre diameter during an electrospinning process.

ad c) Identification of flow conditions of compressible and incompressible fluids in nanoscale structures

The effect of DC voltage and a fluid polarity on the fluid permeation through carbon nanotube membranes

The expected effect of DC voltage and a polarity on the permeability of compressible fluids (vapours) through conductive carbon nanotube membranes (CNMs) was proved. Precisely, a flow through CNM is among others controlled by the molecular interaction between the fluid and the carbon surface. As a consequence, it was found the permeation of non-polar hydrocarbons exceeded permeation of polar alcohols. The proposed explanation is related to hydrophobic surface of carbon nanotubes with a strong preference of adsorption of hydrocarbons over alcohols and following surface diffusion of hydrocarbons, which contributes to their transport down the concentration gradient. The degree of investigated fluid permeation across CNM changed when the membrane was subjected to a DC voltage. Always, when a voltage was applied, a sudden increase of permeation was observed a vice versa. However, the polar fluids showed now a higher permeation increase than the non-polar ones, what is the opposite result to voltage-free case. The alcohol permeations were up two-fold higher than the corresponding permeations for carbohydrates at the same membrane voltage.

Consequently, the practical outcome of the finding of interconnected effects of fluid polarity and electrical charge on the membrane permeation is a wide range of potential production possibilities to tailor specific membranes for industrial applications.

Monomer-epoxy resin infiltration through the carbon nanotube network

Monomer-epoxy resin flow through carbon nanotube network embedded in polyurethane membrane was governed by a vacuum pressure infusion and monitored by the network electrical conductivity. The aim was to determine a correspondence of fluid motion parallel to the flow through various types of form reinforcing textiles with predictable infiltration patterns to which the network was attached. The obtained results confirmed negligible difference in flow resistance of the network and reinforcing textiles. Thus, the network enabled to monitor the flow front as it penetrated through the reinforcing textiles with sufficient precision. It proved that the carbon nanotube network, for the first time introduced to function in a fluid environment under electricity, is capable to measure fluid flow and provide data for a physical understanding of processing of textile reinforced polymer composites. It was also proved that when the carbon nanotube network is integrated with reinforcing textiles, the network can register the monomer-epoxy resin curing process and finally also deformation of the composite products, when exposition to high loads affects its integrity and structural health.

Adsorption of vapours to electroconductive carbon nanowall structures

The reason to study the adsorption of polar and non-polar compressible fluids (vapours) to the surface of carbon nanowall (CNW) structures was to find out the effect of an arrangement of CNWs on adsorption. The maze-like electroconductive structures consisted of vertical CNWs deposited on silicone substrate with different average distance. The conductivity measurement proved that the structure of nanowall distance 100 nm adsorbed in average more polar and non-polar vapours than the structures with larger nanowall distances. Similarly, this prevailing ability follows also from the comparison of carbon 100 nm vertical nanowall structure with the vapour adsorption in the chaotic nanowall arrangement structures and carbon nanotube structures. Hence, a justified practical result is that the nanowall adsorption properties can be controlled by the distance of nanowalls within the adsorbing structure.

The adsorption of vapours onto the carbon nanotube network surfaces and its effect on the thermoelectric power generation

Adsorption of various compressible fluids (vapours) on carbon nanotube (CNT) networks was analysed by means of Fourier transform infrared spectroscopy and X-ray photoelectron spectroscopy to get information on the functional groups attached onto the nanotube surface. Without adding a functional group to CNT surface, the adsorption of non-polar vapours (heptane, toluene) exceeded adsorption of polar alcohol (ethanol) onto the CNT surface, which is a similar result as for the effect of polarity on the vapour permeation through CNT membranes. However, when new oxygen-containing functional groups were added onto the CNT surface, the surface polarity increased as well as the better affinity of polar molecules (ethanol) to nanotube surface, which enhanced the polar vapour adsorption over the adsorption of non-polar vapours. Moreover, it was found up that the oxygen-containing groups enhanced thermoelectric power generation (TEG) of CNT networks. When this phenomenon is combined with the vapour adsorption onto CNTs, the TEG can be controlled by vapours. However, the other way around, TEG can function also as a self-powered

thermoelectric vapor sensing element where the source of waste heat supplies electricity to detect the adhesion of ambient vapours. Nevertheless, the interaction between electrical properties of CNT network and adsorption of vapours onto CNT surface has further potential applicability. For instance, it was found, when the antenna with a radiating microstrip made of CNT network structure is exposed to various vapours, the antenna radiation can be modified by adsorb vapours or vice versa, the antenna can provide remote detection of ambient vapour presence.

ad d) Development of advanced theoretical methods for flow-field analysis

Modification of the widely used vortex-identification Q-criterion

Modification of the widely used vortex-identification Q-criterion has been proposed. Recall that the original Q-criterion defines incompressible vortices as the regions in which the vorticity magnitude prevails over the strain-rate magnitude. The proposed modification takes into account compressibility by using the principal strain-rate difference vector. The magnitude of this vector is quite analogous to the well-known scalar quantity, the so-called equivalent (or von Mises) strain rate, which is responsible for the shape deformation of a fluid element and apparently independent of volumetric changes. The proposed modification can be interpreted in terms of corotation of line segments near a point in strain-rate principal planes. The modified Q-criterion produces less noisy outcome (i.e. less contaminated by shear) as shown for a reconnection process of two Burgers vortices, a flow around an impulsively started flat plate at an angle of attack, and a 3-D transonic flow past a turbine cascade.

Relating vortex to the balance between vorticity and strain rate

A new analysis of the vortex-identification Q-criterion and its recent modifications has been presented. In this unified framework based on different approaches to averaging of the cross-sectional balance between vorticity and strain rate in 3D, new relations among the existing (recently published) modifications have been derived. In addition, a new method based on spherical averaging has been proposed. It is applicable to compressible flows, and it inherits a duality property which allows its use for identifying high strain-rate zones together with vortices. The new quantity has been applied to identification of vortices and high strain-rate zones in a flow around an impulsively started flat plate at an angle of attack, in a flow past a sphere, and for a reconnection process of two Burgers vortices.

Stretching response of Rortex and other vortex-identification schemes

As the benchmark input of the velocity-gradient tensor for investigating the stretching response, a uniaxial stretching coupled with an inevitable uniform radial contraction for incompressible flow has been considered while assuming the vorticity vector aligned with the stretching axis. A straightforward comparison of the stretching response for several popular vortex-identification criteria and the recently proposed vortex vector (Rortex) has been presented. In addition, the outcome of the triple-decomposition method in terms of the residual vorticity tensor has been employed due to its planar coincidence with Rortex. The stretching sensitivity of the examined schemes significantly differs and, consequently, reopens the persisting vortex-identification problem that the requirement of orbital compactness of the motion inside a vortex contradicts with the allowance for an arbitrary axial strain.

Regularity criteria in terms of two vorticity components

The fundamental questions concerning the regularity and uniqueness of weak solutions to the Navier-Stokes equations still remain open. One branch of the present investigation is the conditional regularity: it is supposed a priori that the solutions are endowed with reasonable additional properties and the regularity is proved. The uniqueness then follows immediately. It has been known since 1999 that the solution (velocity plus pressure) is regular (smooth) if two vorticity components lie in a suitable Lebesgue space. Using the Biot-Savart law and suitable form of the Bony decomposition this result has been generalized to the Besov spaces. The Besov spaces give a good insight into the frequencies of the solution, the Bony decomposition serves as a tool for the study of the interactions of the low, middle and high frequencies of the flow. The Biot-Savart law translates the properties imposed on the vorticity to the whole velocity gradient. The results are optimal from the scaling point of view (Prodi-Serrin level 2).

Regularity criteria in terms of one velocity component, the gradient of one velocity component, one (diagonal or non-diagonal) entry of the velocity gradient or several entries of the Hessian tensor

Suitable estimates of the nonlinear convective term form one of the main obstacles in the study of the regularity are. Here one relies mightily on the Troisi inequality which can be understood as a certain generalization of the standard Sobolev inequalities. It provides the estimates of the Lebesgue norms of functions with the Lebesgue norms of their partial derivatives where the individual partial derivatives generally assume different Lebesgue exponents. Several generalizations of the standard Troisi inequality have been proved for the case of anisotropic Lebesgue spaces. The various versions of the generalized Troisi inequality are effective tools for the study of the conditional regularity, where different velocity components or entries of the velocity gradient are endowed with different additional conditions. As a result several non-optimal regularity results in the frame of Lebesgue spaces and some almost optimal results in the frame of anisotropic Lebesgue spaces have been obtained. The results in terms of one diagonal entry of the velocity gradient are generally better than the results in terms of its non-diagonal counterpart.

Regularity criteria in terms of one directional derivative of the entire velocity field

In this case one further generalizes the Troisi inequality with partial derivatives of powers of functions on the right hand side of the inequality. Together with the use of anisotropic spaces it then leads to very tedious elementary computations, nevertheless the optimal regularity is obtained up to the endpoint Lebesgue spatial exponent 3/2. For the exponents greater than 3 a non-optimal regularity criterion has been obtained.

Regularity criteria for magnetohydrodynamic equations

The methods developed for the case of the Navier-Stokes equations have been applied to the three dimensional incompressible magnetohydrodynamic equations. Here the study of the mutual interplay between the magnetic field and the fluid velocity and pressure is the crucial part of the research. If the gradient of the vertical velocity component and the horizontal magnetic field satisfy certain integrability conditions with respect to space and time variables in Lebesgue spaces, then it has been proved that the weak solution is regular.

ad e) Hydrodynamic interactions in particle-laden flows and mixing reactors (both in terms of experimental and numerical approaches).

Slurry flow behaviour in inclined pipe sections

The effect of pipe inclination, mean transport concentration, and mean velocity on flow behaviour of settling slurries was investigated in an experimental pipe loop with inclinable pipe sections. The flow characteristics were studied for fine glass beads-water slurries and for medium-to-coarse sand-water slurries. The concentration profiles showed different degrees of stratification for the positive and negative slopes of the pipe. Frictional pressure drops in the ascending pipe were higher than those in the descending pipe, the difference decreased with increasing flow velocity and inclination. It was found that the Worster-Denny formula overestimates the frictional pressure gradient in an ascending flow. For fine-grained settling slurry the effect of the hydrostatic component of the pressure drops becomes more significant than the effect of the frictional pressure drops. A new method, based on gamma-ray detection, was introduced to detect the deposition limit by sensing a change in the local concentration. The deposition limit velocity was sensitive to the pipe inclination, reaching higher values in the ascending than in the horizontal pipe, the maximum was reached for an inclination of about +25 degrees, and then the limit remained practically constant, about 1.25 times higher than that in the horizontal pipe.

A layered model for inclined pipe flow of settling slurry

A new layered model was proposed for flow of heterogeneous slurries in inclined pipes. It predicts the concentration distribution, pressure drops (total, frictional), and velocity of particles sliding along the pipe invert. The model recognizes a bed layer in which particles are in mutual permanent contact and their concentration distribution is uniform, and the interfacial shear layer, which contains particles in sporadic contact. For a given pipe inclination, the model predicts the deposition limit velocity, and for other flow velocities the profile of solids distribution, pressure drops, and sliding bed velocity. The model is capable to predict successfully the experimentally observed trends exhibiting that descending flows produce higher frictional pressure drops and are more stratified, with faster sliding particles at the pipe bottom, than ascending flows at the same flow conditions. The model provides more detailed information on the effect of pipe inclination than the classical formula by Worster and Denny.

Computational investigation of fine glass-bead slurry flow in horizontal pipe

Numerical simulations have been carried out regarding the turbulent flow of glass beads in a horizontal pipe, for slurry velocity up to 4 m/s and four overall volume concentrations up to 35 %. Use is made of the extension of the Eulerian, two-fluid, Inter-Phase Slip Algorithm of Spalding to dense liquid-solid flows. The model predictions of pressure gradient and concentration profiles were validated against measurements. The numerical results provided clearer insight into the fluid dynamic behavior of the slurry. Particularly, the effect of slurry velocity and overall concentration on the mean velocity profile of the solid phase and the slip velocity was discussed.

Mixing characteristics in a vessel stirred by a radial impeller - comparison of experimental and numerical approaches

The hydrodynamic interactions of a turbulent flow and a Rushton impeller inside an agitated tank reactor were investigated both experimentally and numerically. Angle resolved Particle Image Velocimetry (PIV) technique with an angular displacement 0.3° has been applied for different values of Reynolds number. In the vicinity of the blades

several planes oriented in the radial, tangential and axial directions were measured so that all velocity components were determined. PIV-based results were compared to those obtained by Detached Eddy Simulation (DES). It was showed that the Detached Eddy Simulation is a suitable tool to predict the turbulent flow inside the tank stirred by a Rushton turbine.

Radial impeller jet analysis using a semi-analytical method

On the basis of the conventional turbulent jet theory and the general theoretical framework of scalar dispersion in turbulent shear flows a novel formulation of the radial impeller jet in stirred tanks was determined. Whereas previous studies considered the impeller jet as developed, the new approach considered two separate spatial regions along the radial axis: the zone of flow establishment (ZFE) and the zone of established flow (ZEF).This formulation is accompanied with semi analytical expressions for the prediction of turbulent key parameters including the random part of kinetic energy and kinetic energy dissipation rate in the ZFE. The new theoretical framework is validated both with laser Doppler anemometry measurements and with 3D numerical simulations using a standard turbulent model. Since the proposed model is scalable it is well suited to a variety of industrial applications.