E. SCIENTIFIC, TECHNOLOGICAL OR INNOVATION EXCELLENCE

33. Presentation of the research programme P2-0196 for evaluation according to the criterion of Scientific, technological or innovative excellence

Description of the research programme with regard to state of the art in the field of Power, Process and Environmental engineering

Analysis, development and optimization of characteristic engineering systems in the area of power, process and environmental engineering can only be successful if fundamental physical phenomena within machines and devices are well understood, as well as effective and innovative numerical methods combined with experimental methods are developed and regularly improved. In this field of research transport phenomena in fluids and solids with emphasis on multi-component multi-phase reactive flows present the main experimental and computational challenges. The basic scientific theoretical tenets of the proposed engineering research program are therefore transport phenomena in solids and fluids, i.e. transport of momentum, heat and mass under prevalent turbulent fluid flow conditions. Among research techniques for assessing these problems, the Computational Fluid Dynamics (CFD) has become an indispensable scientific and engineering tool enabling closer insight into spatial and temporal process characteristics. Using CFD methods for accurate computation of transport phenomena in multi-phase and reactive multi-component flows heavily depends on the models used, as these models describe physical phenomena which at a present state of the art cannot successfully be derived from the first principles. Whether such models may indeed be used with confidence in results depends on a multitude of parameters, however. Specific models cannot be generalized but had to be tailored to some extent to particular types of transport phenomena and range of operating conditions of machines and devices. The development of specific computational models typically relies on some basic computational platform, i.e. a CFD computational code in the case of transport phenomena in fluids and solids. Typically, high-end engineering design is based on vendor codes with predefined physical models, however, to reach the state of the art computational levels improvements to existing models or development of new models are necessary. In the proposed research, the latter will be done on the level of vendor codes (Ansys CFX/Fluent, AVL Fire), on the level of open source codes (OpenFOAM) and on the level of in-house developed computational CFD tools, based on the variants of the Boundary Element Method (BEM). As the proposed research programme consists of three major engineering application areas and the area of development of targeted innovative computational tools on the basis of the BEM, in the following a brief description of the state of the art at selected research fields with respect to research goals of the proposed programme will be given.

The Boundary Element Method (BEM) [1] is a powerful technique used to solve partial differential equations (PDE). It relies on the use of Green's second theorem and the knowledge of the fundamental solution of the underlying problem to establish an integral formulation, which depends solely on the boundary unknowns - the unknown function and its normal derivative - flux. Thus, in order to find a solution of a PDE, BEM requires integration only over the boundary of the problem domain. The main drawback of the method is the fact that matrices in the final system of linear equations are fully populated. Several techniques have been proposed to accelerate the solution of boundary integral equations [2, 3] such as the panel clustering method, the fast multipole method, wavelets, adaptive cross-approximation (ACA), and hierarchical $\mathcal{H}$ matrices. These approaches are all aimed at reducing the storage and computational cost from $O(n^2)$ to $O(n \log n)$ or $O(n)$, however with ever-growing demands on the grid density and temporal resolution there is still the need to further improve these approaches. As one of the major application fields will be the computational analysis of dispersed multiphase flows by means of particle point source approximation, the BEM based numerical model offers some major advantages over established approaches [4–6], which model the interphase exchange terms by an introduction of some simplifications to the Dirac function. In the case of the BEM, the numerical treatment of point-wise sources is numerically sound and extremely accurate since in the integral forms of the energy, mass and momentum conservation equations, the effect of particles, included in a domain integral, is transformed into a simple operation of addition without any approximations used.

Dilute dispersed two-phase flows, where point source approximation of a particle's interaction with the fluid phase is the method of choice, are often encountered in process, power and environmental engineering with a typical problem of a micro size solid phase dispersed in a continuous fluid phase. In order to accurately predict particle trajectories within the fluid flow the Euler-Lagrange model, which considers the fluid as a continuous phase in interaction with the solid phase in form of a collection of individual particles of different sizes, shapes and densities, physically correct and numerically accurate models of fluid flow - particle interaction have to be applied. On the basis of the previous research [21, 22], it has been shown that the addition of nanoparticles to pure liquid has a key effect on its conductive ability [40], which can significantly improve the efficiency of many technological processes in the field of process engineering. The studies carried out so far have been based on the use of a mathematical model, where the nanofluid is described as single-phase fluid and any interaction between the nanoparticles and the liquid is ignored. Such a model is suitable for dealing with suspensions where nanoparticle concentrations are no higher than 5%, but at higher nanoparticle concentrations the mixture should be treated as a two-phase fluid and the interaction of the liquid and solid phase have to be modelled [18, 19]. Apart from dilute multiphase flows, dense particle-fluid flows are also encountered in numerous processes. For example, in the pharmaceutical industry, there is a need to optimize the tablet coating process by mixing the tablets inside the rotating drum, spreading the liquid medium and simultaneously drying with the air flow [41]. Since the tablets are coated with a suspension in a rotating drum, with solvent evaporating from the surface of the tablets in contact with heating air, it is necessary to simulate the fluid flow and particle-particle interaction as accurate as possible. Recently, the coupled solution of the problem by means of the Discrete Element Method and the Computational Fluid Dynamics solvers is gaining attention [42], however, there are still many open questions regarding correct modelling of particle-fluid interaction. The majority of available models are valid for single particle-fluid flow case.

In recent years, the study of heat transfer in biological systems, such as human tissue, as a basis for the development of new diagnostic methods based on computational models and experimental data for determining abnormalities in the body or the observed tissue, is gaining interest. The new methods are based on the determination of the temperature distribution in the observed tissue, which is directly related to the physiological or pathological changes, which are the cause for changes in the measured temperature. With the development of thermographic cameras as well as numerical methods, thermography has recently become an interesting non-invasive technique for various medical applications, such as breast cancer diagnostics, vascular diseases, diagnostics in dentistry, skin diseases, blood pressure monitoring, etc. [23, 24]. In this works, thermography is divided into a static and dynamic part, with the latter having significantly more advantages than the static one, which means it is becoming important not only for the scientific research but also for the practical use. In dynamic thermography, the observed tissue is stimulated by heating or cooling for a certain period of time, whereby a temperature response is recorded, which gives more valuable information about the observed tissue response than the static temperature distribution [25–28]. Also, the recorded temperature response can be used to determine important parameters from the medical point of view, such as the size of the affected area, invasiveness, depth, etc. The research in this area can be further extended to the field of heating, ventilation and air conditioning with an emphasis on comfort factors [30], as the thermal conditions in closed spaces (offices, flats etc.) have a direct impact on the of blood flow through the tissue, and its reactions to external stimuli, which could lead to advanced thermal comfort computational models taking into account an active response of the occupants.

In spite of modern alternative vehicle drives, according to experts, a vehicle with an internal combustion engine that uses modern exhaust gas treatment systems [33], is much more favourable to the carbon footprint than an electric vehicle. Therefore, it is still reasonable to further develop internal combustion engines, both forced-ignition and self-ignition engines, as their modern emission performances do not differ significantly. In this view, hybrid fuels, used in a combination of electric and internal combustion engines, play an important role in reducing environmental pollution, with a large impact on urban emissions reduction [34]. To optimize the performance of hybrid vehicles and lower their environmental impact, further progress in the development of internal combustion engines is still indispensable [35] and can additionally contribute to the reduction of emissions. It is also important to emphasize the great potential of internal combustion engines for the energy use of biomass and waste materials [36]. Their important advantage over other combustion methods is the high thermal efficiency in a wide power range, which ensures high flexibility of use and efficient application in the context of the rational use of alternative energy sources. In the latter view, combustion of solid fuels on a grate with a separate air or fuel supply is a method by which pollutant production, resulting from both complete and incomplete combustion, can be effectively reduced. The effectiveness of such systems depends on both process and geometric parameters [49]. Such combustion systems represent the complex influence of geometric and process parameters on the formation of pollutants [51], which has not yet been sufficiently researched. Numerical modelling offers an efficient tool for analyzing such systems since it enables fast adaptation of both geometric and process parameters, which allows parametric studies and the determination of the influence parameters on the combustion process [31, 50].

In hydromachinery, the problem of cavitation occurs on many scales, both in space and in time at different operational regimes. Today the general consensus is that the formation of the damage is a result of a consequence of several events, with the collapse of the vapour phase as the critical event. It is generally acknowledged that the collapse of the cavitation cloud causes a shock wave which interacts with single cavitation bubbles that are present in the vicinity of the wall [43] and causes pits. The following general questions remain open: how exactly a cavitation structure collapses, how generated pressure pulse initiates the erosion, how does a pit develop. The state of the art in CFD research [44, 45] is focused on models for cavitation erosion prediction. In [48] cavitation in a Pelton turbine was studied with the outcome that the cavitation results in erosion of material only if the vapour is stuck to the bucket and the condensation process is very fast without the presence of air.

Objectives of the research programme with respect to originality of the research and its impact on development of new research directions

In **Objective 1** the field of **advanced numerical models for computation of two-phase flows** further development and advanced application of novel interaction models for numerical simulation of dilute dispersed two-phase flows by the Lagrange-Euler approach will be conducted. The first part will be devoted to advanced validation of the novel shear-induced lift model [9, 10] by means of DNS as well as improvement of the Stokes drag force model on ellipsoids for the case of intermediate or high Knudsen number flow regime, that occurs in the case of microparticles. Furthermore, since advanced application of the developed models for the case of flows in narrow channels (the lung case) is one of the objectives, where interaction with the wall as well as regions with higher particle densities occur, the models for non-spherical particle interaction with the wall will be studied and extended to in-flow particle-particle collision of non-spherical particles. Due to the anisotropic shape, the model for non-spherical particle deposition on a wall has to accurately detect the colliding point between the particle and the wall, for which we plan to develop a computationally efficient algorithm by adopting the idea of multi-level grid refinement, Fig. 1. This has to be followed by the calculation of the adhesion force and the resistance force acting on the particle during the colliding process, where we will, in collaboration with prof. Steinmann from the University of Erlangen-Nuremberg, Germany, further continue to develop the model of Cui & Sommerfeld [11] and make it applicable to the case of non-spherical particles and walls with a thin liquid layer (the case of lungs). Since in-flow particle-particle collision of non-spherical particles can occur in local regions of otherwise dilute particle flows, the novel colliding point determination model will also be extended to the case of colliding of prolate ellipsoids in the three-dimensional space.

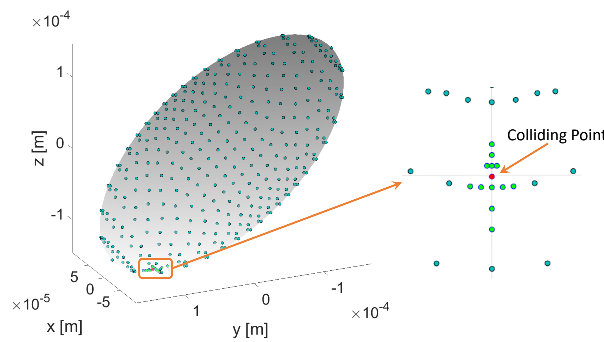

Figure 1: Illustration for the use of multi-level grid refinement to determine the colliding point between a prolate spheroidal particle and a plane wall ($a = 100\,\mu m$, $\lambda = 2$, Euler angle= $[0,\, 52^\circ,\, 0]^T$, three refinement levels are applied).

Furthermore, a novel force model for particle-fluid interaction of a porous permeable ellipsoidal particle with inhomogeneous mass distribution (sludge floc case, Fig. 2) will be studied. Finally, detailed analysis of dynamics of non-spherical micro-sized particles arising in process and environmental engineering will be studied, which include sedimentation of non-spherical porous particles with inhomogeneous mass distribution in a typical secondary wastewater clarifier, active biomass granule settling.

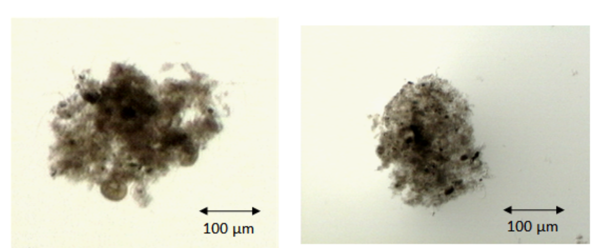

Figure 2: Typical shape of sludge flocs originating from municipal wastewater treatment plant.

In many industrial and environmental cases, the size of the particle in question is very small. This can lead to the case, where the continuum hypothesis, on which the governing equations of fluid motion are derived, is no longer fully valid. In such cases, the Stokes drag force models, which rely on the no-slip boundary condition for the fluid at the particle surface, are no longer accurate. The typical modelling solution is correcting the classical force models with the Cunningham slip correction factor, in order to account for non-continuum effects when calculating the drag on small particles. As the particles under study will be non-spherical, the correctness of the Cunningham slip correction factor, developed for spheres, has to be verified. For this case, a DNS of flow around the ellipsoidal particle by implementing the slip velocity boundary conditions in the form of the Maxwell model will be performed. The Finite Volume Method based fluid flow solvers, as well as the BEM based fluid solver, will be used. The main advantage of using BEM as the fluid flow solver lies in the unique feature of the BEM solver, where flow results at the solid boundary for function (velocity) as well as function normal derivative (velocity derivative normal to the boundary) are obtained in a single computational step, without any numerical differencing schemes. Since in the DNS the slip boundary condition at the wall builds on the velocity derivative normal to the boundary (the Maxwell slip model), this would allow an efficient and accurate computation of the drag force, exerted on the particle, under conditions of higher Knudsen number flows, and hence calculation of the correct value of the Cunningham slip correction for ellipsoidal particles.

In **Objective 2** the Eulerian part (fluid flow) development of a **novel point source particle-fluid interaction model** in the context of the Boundary Element Method and related techniques will be developed, which can be applied to momentum transfer as well as heat and mass transfer from moving particles in a fluid flow. This greatly simplifies the implementation of a two-way coupling approach, however, the term added due to the effect of particles, is inversely proportional to the distance from the particle location to a computational grid node. Although, theoretically, this singularity does not cause any problems, when implemented in a solver using single or double precision arithmetic, rounding errors do occur. When the particle approaches the grid node, the large value of the term causes the numerical model to be unstable. Finally, the fluid flow and particle tracking solvers will be improved in terms of computational efficiency by the development of the adaptive cross approximation technique and hierarchical $\mathcal{H}$ matrices. The developed models and techniques will be validated on several test cases, including non-spherical particle transport in direct numerical simulation (DNS) of channel flow and sedimentation of porous sludge flocs.

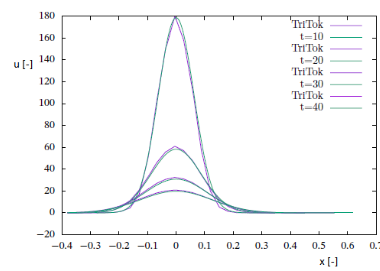

Figure 3: Comparison of analytical and numerical solution for a temporal development of the field function u due to the point source in a stationary flow.

In **Objective 3 transport phenomena on particles in process flows**, important in the development of many process devices, including devices used in coating and drying processes and pulmonary delivery of drugs, will be studied. In the pulmonary delivery of drugs regional deposition effects are important in order to understand and control optimal drug delivery in the form of microscopic particles. Up until now, most studies of the particle transport and deposition in human respiratory airways focused on spherical particles [14], however, most spray-dried aerosol drugs are non-spherical, which can be modelled in the shape of prolate spheroids or fibres. There have been only a few studies that reported on fibre deposition in human respiratory airways, therefore we plan to perform numerical simulation of the human respiratory airway and verify the obtained numerical results with the experimental measured data [7], in order to establish an accurate Lagrangian particle tracking code for micro-sized drug delivery in the human respiratory airway. Here, the established cooperation with Dr. Lizal and Prof. Jicha from Brno University of Technology in the Czech Republic, who developed a physically realistic replica of the human airways from the oral cavity to the 7th bronchial generation [15] as shown in Fig. 4, will be used. In modelling of drying the three stage drying model will be further improved by introducing the Boundary Element

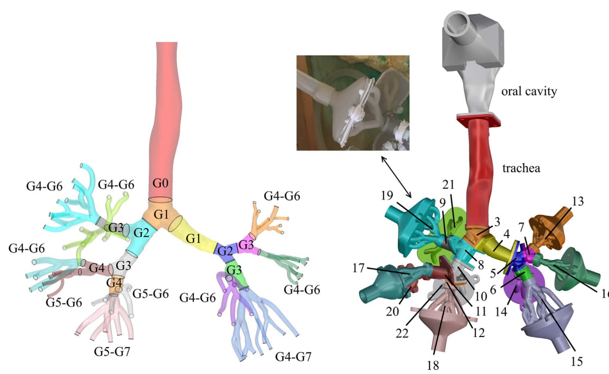

Figure 4: The geometry of respiratory airways with generations of bronchial branching for individual segments (left); segmented replica for deposition experiments (right) with the photo of connection to the rest of the experimental setup [7].

solution of the heat and mass transport in the interior of the particle, resulting in lowering of the computational demand of the spray as well as fluidized bed drying model. In the field of dense particle-fluid flows, the aim of the research is to implement and upgrade a coupled CFD-DEM numerical simulation based on vendor CFD codes (AVL Fire, Ansys Fluent) and DEM codes (EDEM), which will be capable of an accurate solution of the tablet drum coating process [52]. A targeted analysis of the influence of the process parameters on the final quality of the tablet coating will be performed, and an integral model for engineering calculation of the coating efficiency will be developed. For the purpose of validation, a dedicated laboratory drum coating device will be constructed and used for validation of the computational results.

Objective 4: As the governing equations of transport phenomena are inherently nonlinear, unsteady and inhomogeneous, **development of BEM to unsteady and inhomogeneous transport problems in fluid flows** is currently still a subject of intense research [39] as the problem of variable diffusivity and fluid velocity presents a challenge for the use of BEM with fundamental solutions dependent on these parameters. We propose to develop a method, which will be able to handle variable material properties in a fast and efficient manner. The main focus of its application will be in the computation of transport phenomena in porous media saturated with nanofluid [22]. The nanofluid flow model will be based on a two-phase computational model, also known as the Buongiorno model [17, 18]. The Buongiorno model takes into account the interaction between nanoparticles and the fluid phase, which can be described by one or more mechanisms, such as, for example, Brown's diffusion or thermal diffusion. The basic, single-phase mathematical model will thus be extended by taking into account the thermal diffusion of the nanoparticles in the fluid, as well as by specification of the additional model parameters in the Brownian motion model.

In **Objective 5** the field of **environmental engineering transport of particulate phase in fluid flows** will be in the centre of the investigation. One of the most notable systems is the secondary clarifier in a wastewater treatment plant, Fig. 5. There exist many research articles dealing with Lagrangian particle tracking with CFD based design of a secondary settling (sedimentation) tank, where sludge particles are treated as hard spheres with size-independent properties and simple resistance models, aimed at mimicking the porous structure of the flocs [13, 16]. Such models lead to over-prediction of sludge floc sequestration and are therefore not recommended for an accurate sedimentation analysis. Our aim is to implement the derived Stokes drag model for porous non-spherical particles as well as the new shear lift models in the Lagrangian particle tracking model for turbulent flow, resolved by the CFD computation, and compare the results with published results in the scientific literature. A sensitivity analysis of the floc settling behaviour under various flow conditions by using the developed models will be studied, which will be further extended to the comparative study of the performance of hard sphere based sedimentation models and porous non-spherical sedimentation models for the case of typical flow conditions in sedimentation basins. Also, the effect of shear lift on sludge floc trajectories will be studied. Furthermore, as a practical application of particle-fluid flows, we plan to develop a model of sediment transport in estuaries and other types of surface water flow, which can be considered as a special case of a porous media where the solid phase is not fixed but changes its position in space and time [20]. This is a significant problem of sediment displacement, caused by fluvial surface erosion, in surface water flows caused by the action of water currents, which is still a practical problem in terms of hydraulic design as well as a modelling challenge in terms of physical modelling. The model parameters of the moving porous substance will be calibrated in the case of certain types of surface water flows with experimental procedures for the determination of the concentration of particulate matter in the water flows.

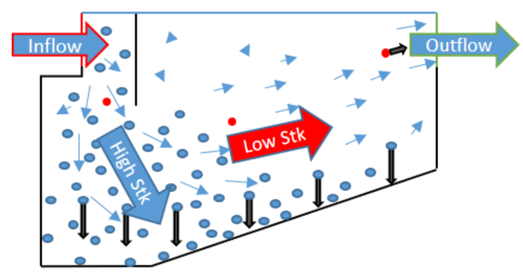

Figure 5: A schematic representation of flow conditions and sedimentation of particles with low and high values of Stokes number in a typical secondary clarifier geometry.

Objective 6: In **thermal engineering research** will be focused on development of computational model for full scale numerical simulation of the process of vial lyophilization, including heat and mass transport inside the vial under extremely low system pressures and low temperatures, as well as CFD simulation of vapor transport in the drying and condenser chamber of pilot scale and industrial scale lyophilizers, with a continuing strong collaboration with the pharmaceutical sector (LEK/Novartis). Also, computational tools for accurate determination of lyophilization design space will be developed. In the field of dynamic thermography development for medical applications has not yet reached its end, as there are still many unknowns and obstacles for its practical use. Thus, it is necessary to work on the development of not only the experimental thermography technique but also in the numerical field, with a special emphasis on the development of optimization techniques for solving direct and inverse problems, [29]. Thus, the research work will focus on the development of the numerical methods and new approaches for the use in dynamic thermography, with the aim of increasing accuracy and speed of numerical procedures, in particular using the Boundary Element Method. Also, the research work will be directed towards the development of the devices necessary for a successful application of the dynamic thermography. One of such devices is a device for controlled cooling or heating of tissues, which represents a novelty, as well as the development of dedicated computer software for analyzing thermographic images. The originality of this work will not only be rooted in the development of a new hybrid experimental-computational method for the use in medical applications, but also in the development of fast numerical techniques based on the Boundary Element Method, where a boundary only domain discretisation can be used, in the development of new targeted numerical techniques for solving inverse problems, as well as in the development of new dynamic thermography equipment with the goal of achieving as controlled cooling and heating procedures. The developed experimental controlled cooling/heating device will be used to validate the developed computational tools as well as for the purpose of evaluation of some of the important tissue parameters used in the medicine. In addition to this, the work on the use of perfusion flow models and human comfort factors, as well as analyzing the phenomena in greenhouses in terms of improving plant growth, will be continued.

In **Objective 7** the field of **reactive flow dynamics of combustion processes** will be covered with the development of numerical models for studying the combustion process of solid fuels in small-scale and plant scale appliances, where separation of air and fuel supply is implemented, Fig. 6. The aim of the research work is to develop a method that will enable the study of the influential factors on the production of pollutants in combustion systems with the separate supply of combustion air and fuel (air and fuel staging). For this purpose, an existing one-dimensional empirical model for combustion will have to be upgraded with the appropriate sub-models of the heterogeneous transformation of fuel into gaseous products, as well as mechanisms for the production of pollutants. The research will provide guidelines for the selection of optimal geometric and process parameters for the development of new systems. In the field of internal combustion engines, we will continue to explore the impact of the use of alternative fuels on the characteristics of the injection process, the process of formation and decay of the spray, and the ecological, economic and performance characteristics of the engine. At the same time, we will explore the possibilities of using various new additives to diesel and alternative fuels in order to improve the characteristics of the high-pressure fuel injection systems within the common rail engines [37], [38]. With the use of new additives to alternative fuels optimization of the design and control parameters of the engine and the injection system will be in the focus of our research. Experimental and numerical investigations of the characteristics of the injection and development of conventional and alternative fuel jets of synthesized bio-raw materials or waste materials will be carried out, where a strong collaboration with researchers from the University of Jaen, Spain will be further continued. Modern methods of mathematical programming and experimental research will be used in order to guarantee achieving ever more stringent environmental standards with new alternative fuels.

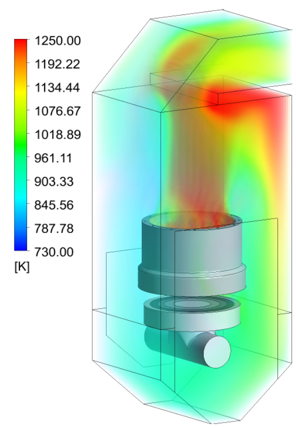

Figure 6: A CFD based simulation of a typical small combustion unit

In **Objective 8 cavitation in hydraulic machines** will be studied with numerical and experimental approaches. Using CFD, we will continue with the numerical analysis of different cavitation regimes (swirl cavitation) with existing algorithms. We intend to further optimize them to achieve better prediction of pressure fluctuations during the implosion phase. After that, we will transfer the results into mathematical models for predicting cavitation erosion. At the same time, we will monitor the state of research in the world and replace the algorithms with new ones that will more universally analyse the exchange of flow variables between the liquid and gaseous phases. In the framework of the experiment, we will use modern visualization techniques to research the mechanisms of the formation of surface damage (pits) at the spots where implosion of cavitation structures occurred. The results of the experimental work will be transferred to the numerical environment. Thus we will be

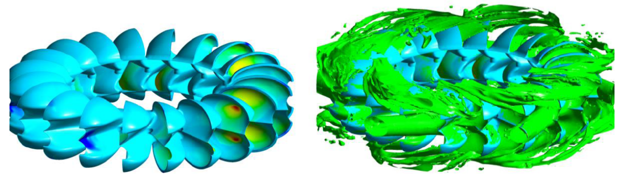

Figure 7: Pressure distribution on the buckets (left) and water jets and evacuating water sheets presented as isosurface of Water Volume Fraction = 0.5 (right).

able to independently validate the developed algorithms or numerical models. For Pelton turbines, cavitation prediction for a prototype cannot be obtained from the results of the model tests. Therefore, numerical prediction of cavitation on a prototype is extremely important. For efficiency prediction with cavitation modelling the domain of simulation will no longer be reduced to five buckets and one jet 7, because in such a way the efficiency cannot be predicted accurately [48]. The domain will be a complete runner (or half of it due to the symmetry) and the jets from all nozzles. In the case of a turbine with more nozzles, the simulations will be especially demanding. Next important issue will be to modify the buckets with the purpose to improve cavitation characteristic without deterioration of the turbine efficiency. The second topic will be a prediction of cloud cavitation in water turbines and pumps. First CFD based results for a centrifugal pump were already obtained, but unfortunately, the simulations were very unstable and extremely long. With such unstable and time-consuming simulations, no useful results can be expected in case of the development of a new machine. We have to determine a numerical setup, which will serve in all cases and will give results accurate enough for practical use. Therefore, the study will be dedicated to determining proper mesh density, turbulence and cavitation models, discretization schemes and time step for accurate prediction of cloud cavitation in a reasonable time.

Methodology

The proposed research will be conducted by a combination of analytical work, development and use of computational methods and experimental work for validation of the developed analytical and numerical models. An in-depth analysis of the state of the art techniques will serve as a starting point in the development of new models. Dedicated in-house computational methods will be derived for the modelling of nonspherical porous particles interaction with the fluid phase, for transport of fuel jet development and simulation of the injection process will be developed together with the use of modern computational codes for simulation of processes in the nozzles, in the case of turbomachinery state of the art cavitation models will be experimentally studied and model constants will be optimized for the use in industrial scale cases. The results of numerical simulations will be validated by the results of laboratory testing. New experimental set-ups will be developed, including transparent drum coating device, small scale waste incineration plant and a new common-rail injection systems test system with open control electronics for selecting injection control parameters and adapted it for experimental monitoring and visualization of injection processes.

Tentative timeline of the proposed research activities

The Table below illustrates the timeline of the proposed research activities.

	Year I	Year II	Year III	Year IV	Year V	Year VI
Objective 1	•	•	•			
Objective 2				•	•	
Objective 3				•	•	•
Objective 4		•	•			
Objective 5				•	•	•
Objective 6	•	•	•			
Objective 7	•	•	•	•	•	•
Objective 8	•	•	•	•	•	•

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F. POTENTIAL IMPACT ACHIEVED BY THE DEVELOPMENT, DISSEMINATION AND USE OF THE EXPECTED RESEARCH RESULTS

34. Presentation of the research programme P2-0196 for evaluation according to the criterion of Potential impact achieved by the development, dissemination and use of expected research results

Importance for the development of science or profession

Understanding and ability of prediction of characteristics of technical systems with prevailing turbulent and multiphase flows is based on deeper knowledge of transport phenomena in these flows. The development of new and accurate methods of computer based simulations of transport phenomena, which greatly exceed the quality of results of classical, on empirical realizations based engineering calculations, is therefore of prime importance for the further development of engineering sciences in the field of power, process and environmental engineering. Here we aim at developing application targeted advanced computational methods for the solution of some complex transport phenomena, for which there exist only partial computational solutions, and at validation of these methods, which will enable the scientists and professionals to perform parametric analyses and optimization of targeted processes.

In the field of development of new numerical methods in the framework of the Boundary Element Method we will develop targeted accurate and innovative models of processes in process and environmental engineering, as well as further improve computer and memory demands of the method. The development of advanced models for heat and mass transfer in dispersed flows will lead to a detailed insight into complex flow, temperature and component (species) fields in heat and mass transfer separation devices, waste to energy plants as well as internal combustion (IC) engines. The main effort will be in developing accurate computational approaches for two-way coupling of particle-fluid flow systems. New computational models of transport phenomena within the particles and porous media will also be developed, including multi-stage drying of porous particles under atmospheric and low pressure conditions, gasification of solid waste particles as well as momentum transfer interaction models for non-spherical porous particles with inhomogeneous mass distribution, as found in separation devices in wastewater treatment systems and bioreactors with active granules.

In the field of the advanced use of numerical methods for computation of flows in turbomachinery the scientific and professional focus is on the study of transient and cavitating flows. With this we will develop new knowledge of different stable (partial loading, optimal working point, full power) as well as unstable operating regimes (start, runaway), which will be transferred to optimization of model parameters of cavitation models and cavitation erosion models for the broad spectrum of hydraulic turbines, including the Pelton turbine. Based on increasingly rigorous environmenal legislation and the problems in the use of fossil fuels there exist a need to search for new methods of use of alternative fuels in internal combustion engines. The newly developed mathematical models for numerical simulation of injection process and combustion will reduce excessive experimental testings and enable a faster development of more efficient and environmentally friendly IC motors. The equilibrium model of multistage gasification of solid waste on a grate will further be improved to enable a more detailed analysis of combustion characteristics in primary and secondary chamber in the device for thermal use of solid waste. The thermography based analysis of heat transfer in heterogeneous media with partially unknown thermal properties, for which new computational approaches to solution of inverse problems in heat transfer will be developed, will also be extended to interdisciplinary fields, including diagnostic methods in medicine.

Potential impact on economic development

The results of scientific work can in a large extent be directly implemented in advanced design of machines, devices and processes in various industrial subsectors in Slovenia, but also abroad. Here, the research programme members will further strenghten existing scientific and professional collaborations with pharmaceutical industry, home appliences industry, automotive lightning industry, waste-to-energy based power engineering companies, producers of turbomachinery and hydro power based energy providers, where newly developed experimental and computational methods will be implemented for development and optimization of new products and processes. For example, process engineering and pharmaceutical industry in Slovenia but also abroad show large needs for numerical modelling of transport phenomena in dispersed phase of solid particles as well as in modeling of lyophilization. As an application example spray drying of solid particles in flow of continuous fluid (drying air) with three stage drying can be implemented to better predict and improve the energy demands of the process. Also, computational model of virtual industrial scale liophilizator will be developed. Another potential impact can be found in the use of advanced computational tools for heat transfer and mass (moisture) transport modelling in car lightning, in particular as Slovenia features two important manufacturers, one of which (Hella Saturnus) already cooperates with members of our research group. In Slovenia, water power is the most important among the renewable energy resources. Slovenia has a long lasting tradition as well as plethora of knowledge and experience in developing and manufacturing of water turbines with emphasis on Kolektor-Turbointitut, our partner in the research program. If results are to be used in the market one need exceptional characterics of machines and reduction of cost. Both can be achieved with development of new computational methods for high end computational analysis of flow phenomena in water turbines. In the case of smaller commercial projects where manufacturing of physical models is not justified through the cost of the project, the only viable alternative is a dedicated computational analysis with a check of the requested turbine characteristics. In the environmental engineering research focus will be on development of computational methods for thermal conversion of waste, which will be used in computational analysis and optimization of process parameters of waste-to-energy plants in Slovenia, as well as in the analysis of alternative fuel suitability, manufactured either from wood waste or household waste. Multiphase computational methods will also be used for study and optimization of biological process systems (i.e. wastewater treatment plants) as active biological cultures in these flows usually come in form of particles, interacting with flow conditions inside the devices.

Potential impact on social and cultural development

In the area of efficient energy use the research outcomes from subarea of Heating, cooling and climatization (HVAC) as well as from the developed models of natural gas consumption for characteristic groups of consumers will be used for optimization of efficiency of various modes of heating in residential and business buildings while taking into account the local meteorological data. By addressing the issue of thermal conversion of waste we will contribute to understanding, control and improvement of Slovenia's treatment of waste materials, which is currently in a critical phase of development. The thermography based computational and experimental tools for analysis of heat transfer in heterogeneous media will be extended to solution of inverse bio-heat transfer problems, especially for the case of biological tissues, which can be used in early detection of skin melanoma in advanced medicine diagnostics. In the area of academic education, the majority of members of the research team is actively involved in lecturing process at undergraduate and postgraduate studies, thus allowing a fast transfer of state of the art knowledge in the area of power, process and environmental engineering in studies of Mechanical Engineering and Technical Environmental Protection. Internships of students in the participating research group member Kolektor Turboinštitut provide a cornerstone for faster introduction of computational methods to industrial environments, and at the same time result in diplomas, master of science works and doctoral dissertations in the area of numerical analysis of flows in hydraulic machinery.