Fourth Annual PhD Workshop
PhD Study of Mechanical Engineering, Naval Architecture, Aeronautical Engineering and Metallurgical Engineering

Book of Abstracts

July 2, 2018
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Preface

This booklet contains abstracts presented at the 4th Annual PhD Workshop held at University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture, on July 2, 2018. Annual PhD workshop is the integral part of PhD programme of Mechanical Engineering, Naval Architecture, Aeronautical Engineering and Metallurgical Engineering, launched on academic year 2014/15. PhD program is jointly developed by two faculties of University of Zagreb, Faculty of Mechanical Engineering and Naval Architecture and Faculty of Metallurgy.

PhD workshop is aimed to provide forum for exchange of ideas among PhD students, to get most of PhD students at one place and to monitor progress of their PhD theses. Workshop should help students to strengthen their presentation skills and unify quality and transparency of PhD theses produced at different modules of PhD programme. Contributions in this booklet are divided in two broad groups, abstracts of preliminary PhD topics and abstracts of final PhD topics. Former are mostly presented by the first year PhD candidates, while latter are presented by PhD students of second and higher years. Abstract are structured in a way to encourage students to write clearly and concisely purposes of their PhD theses in order to bring their research closer to the wide community and even to those who are not specialists in the field. This booklet could be a valuable and relevant reference for PhD students and their mentors as it represents kind of milestone in the progress of their PhDs. It will also be useful for all stakeholders of PhD education to evaluate quality and progress of PhD theses. Finally, it can be useful for the industry in Croatia as it contains in one place most of the research efforts at two faculties.

20 participants on the PhD workshop presented preliminary topics of their theses, while 26 participants presented final PhD topics. 8 workshop participants belong to the non-academic sector, while 2 among them are from foreign countries (Canada and United Arab Emirates). Contributions collected in the booklet of abstracts are from different modules of the PhD study: Process and Energy Engineering (13 contributions), Computational Mechanics (4), Theory of Structures (8), Mechatronics and Robotics (3), Industrial Engineering and Management (4), Aeronautical Engineering (2), Materials Engineering (2), Advanced Production Technologies (1), Naval Architecture and Ocean Engineering (5) and Metallurgical Engineering (4). Diversity of these topics clearly indicates broad and rich research interests and activities at the Faculty of Mechanical Engineering and Naval Architecture and Faculty of Metallurgy.

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TOPIC NOT APPROVED
Optimization of Dynamic Behaviour of Advanced Active Structures

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Introduction
Inerter is an idealized element in discrete mechanical networks which resists relative acceleration across its two terminals. The coefficient of this resistance is called inertance and is measured in kilograms. A property of inerter elements is that they can be designed and realized in practice having their inertance significantly larger than their mass. This feature is potentially very useful, so that many recent investigations are focused on the realization and use of inerter elements for suppressing mechanical vibrations. The use of inerter elements can be beneficial given the fact that their inertance can be significantly larger than their mass. Consequently a number of new concepts have arisen. These include tuned inerter damper (TID), tuned mass–damper–inerter (TMDI), and inerter–based dynamic vibration absorber (IDVA). Inerter elements can be very useful in both vibration absorption and isolation systems. Dynamic vibration absorbers and isolators can be made active by using inertial actuators with a velocity or velocity + displacement feedback control scheme. In vibration isolation problems it is often necessary to tune the impedance of the isolator elements based on some optimization criteria. This can be done by either minimizing maxima of the response (minimax or $H_\infty$ optimization), or by minimizing the energy in the response signals ($H_2$ optimization).

Aims
Research focus is to analyse the performance of passive and active systems for the isolation of broadband vibrations by using an inerter. Research aims are improving the performance of passive and active vibration isolation systems by using an inerter, and improving the stability of active vibration isolation systems by using an inerter.

Methods
The problem of active vibration isolation with velocity feedback loop will be considered. It will be examined whether using an inerter can improve stability and performance of such active systems in certain situations. It will be examined, by utilizing simplified models, whether using an inerter enables efficient active vibration isolation in group of mechanical systems in which active vibration isolation is otherwise difficult to accomplish: sub-critical group of systems. Subcritical systems are those that have the fundamental natural frequency of a body that is to be protected from vibrations, greater than the fundamental natural frequency of the body that is the source of vibrations. The broadband dynamic excitation of the source body will be assumed. Routh-Hurwitz's stability criterion will be used to determine the stability parameters of the active system. The described method will be applied to a simple two degree of freedom system, so conclusions can be based on analytically derived expressions. Such a simplified system can be considered as a reduced model of potentially more complex structures.

Expected scientific contribution
A new method for improving the performance of passive and active isolators of broadband vibrations by using an inerter will be developed. Consequently, a new method for improving the stability of active isolators of broadband vibrations by using an inerter will be determined.

Keywords
vibration isolation, inerter, active vibration control, direct velocity feedback, stability of active control systems
Numerical Modelling of Surface-Hardened Spur Gear Fatigue Crack Initiation

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Introduction
When it comes to the mechanical power transmission, gears are one of the most commonly used machine elements. Due to the cyclic nature of stresses appearing at the tooth root, material fatigue may occur. It is characterized by the crack initiation near the root fillet area, which may propagate and result in a catastrophic failure of the tooth and the spur gear itself. The tooth root material fatigue, commonly known as bending fatigue, is more prominent for surface hardened spur gears. To gain insight into the location and the number of cycles required for crack initiation, an adequate numerical model predicting the aforementioned is vital. Current numerical and fatigue approximation methods are generally not considering factors such as residual stress, friction, centrifugal force or sub-surface crack initiation. In addition, a distinction has to be made regarding the low-cycle and high-cycle fatigue, whereas some of the methods are more favorable depending on the type of material fatigue.

Aims
The aim of this research is to improve the current numerical and fatigue models, enabling a more accurate prediction of location and the number of cycles required for crack initiation. A resulting model will be applicable to the surface-hardened spur gears. Results will be compared against the commonly used methods for fatigue life predictions. Parameters will be evaluated regarding both the high and low cycle fatigue. Finally, a distinction will be made regarding the surface and sub-surface crack initiation parameters.

Methods
Numerical models generated by employing the finite element method will be used to calculate the stress and deformation values at the tooth root. Strain-life and hysteresis total stress-strain energy methods will be used to predict the location and the number of cycles required for crack initiation. Moreover, power density method will also be considered. The collected data will be validated experimentally, either by using the running gear pair or by performing a single-tooth bending test investigation.

Expected scientific contribution
By including various parameters in the different numerical and fatigue models as well as distinguishing between the surface and sub-surface crack initiation, a more accurate determination of bending fatigue life for spur gears will be possible. Since the results of bending fatigue life predictions will be more precise, they will contribute to an increase of cost-effectiveness of the spur gears. In other words, a premature withdrawal of the operational gear pair as a result of potential crack initiation will be decreased.

Keywords
spur gear, finite element method, material fatigue, crack initiation, surface-hardened gears
The Problem of the Temperature of Stagnation in Solar Collectors

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Introduction
The temperature of stagnation is the temperature a solar collector reaches during peak hours of sunlight if there is no flow through the collector. The lack of flow may be due to a malfunction, or more commonly, due to the fact that there is no demand for heat during that period. The temperature of stagnation in most collector designs can be very high easily surpassing the glass transition temperature of all commonly used mass produced polymeric materials. Historically, this has severely limited the selection of such materials in collector design and kept the price of the collector relatively high compared to what could be achievable. While some solutions have been suggested, currently none of them have provided a widely acceptable solution, especially if passive overheating protection is required.

Aims
Due to the aforementioned problems, the aim is to find a way to passively lower the stagnation temperature in a flat plate solar collector to the point where it will no longer reach the levels surpassing the working temperature of mass produced polymeric materials. This would enable the use of such materials in all parts of a solar collector and make collectors cheaper for the end consumer.

Methods
Based on the performed literature review an initial research was conducted into the behavior of a model polymer collector under stagnation. A model was made and analyzed using ray tracing software. Real optical properties of the material were modelled using theoretical sources and experimental measurements. Measurements were conducted on a makeshift model collector and the simulation model was verified. Based on this the necessary irradiance reductions needed to make polymers viable for use in a collector were determined. In the following steps a number of methods for reducing incident radiation will be analyzed. The method which will be selected will be used to create a full-scale prototype collector.

Expected scientific contribution
The results of this project should provide a concrete method of mitigating the problem of the temperature of stagnation in flat plate solar collectors.

Keywords
temperature of stagnation, solar collector
Categorization of Driving Cycles Considering
Driving Style and Traffic Characteristics

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**Introduction**

Electric vehicles (EV) represent a key enabling technology to make the transport system more efficient, cleaner, quieter, and less dependent on oil reserves. According to the US Environmental Protection Agency, the transport sector was responsible for 28% of the US greenhouse gas emissions in 2011. A significant part of these emissions comes from the commercial vehicle sector, which is illustrated by data showing that between 16% and 50% of total pollutant emissions in transport and between 20% and 30% of the total travels in urban areas, are attributed to freight transport activities. Although the emission of all-electric vehicles is equal to zero, electrified transport can be a viable solution only if the electric energy stored in the EV battery comes from renewable energy sources (RES) such as wind power plants and solar panels. This opens up great opportunities for the development of green transport and energy systems in the future, where, in addition to significant individual developments on the side of EV and RES, advanced information and communication technologies (ICT) also play a key role, including the characterization of traffic situation in terms of a driving pattern identification and prediction of EV arrival at destination time.

**Aims**

The proposed study will focus on the processing and analysis of a large number of recorded driving cycles, synthesis of a small number of representative synthetic cycles, categorization of the driving cycles in real time, and the prediction of EV range, also in real time. The categorization of the driving cycles will take into account the driving style and traffic conditions with the aim of accurate prediction of remaining EV range, and improvement of existing realistic control strategies.

**Methods**

The research will be predominantly numeric, i.e. computer analysis, synthesis and simulations. For the synthesis of the driving cycles the Markov chain method will be used, while different neural network architectures will be used for online categorisation of driving cycles and prediction of remaining EV range. The proposed methods will be implemented and verified through self-developed software tools by using the object-oriented programming languages of C++ and Python. Multiprocessor workstation with appropriate programming support (Matlab/Simulink, Visual Studio, and PyScripter) will be used for research purposes.

**Expected scientific contribution**

A significant contribution will consider the development of a novel algorithm for generating the 3D synthetic driving cycles, that will take into account not only the vehicle speed and acceleration information, but also the road grade, thus resulting in statistically more representative driving cycles than those of lower dimensions, and thereby increasing the precision of the driving cycle categorizations and EV range predictions.

**Acknowledgments**

This work is supported by the EU European Regional Development Fund trough Interreg CE project SOLEZ („Smart Solutions supporting Low Emission Zones and other low-carbon mobility policies in EU cities”).

**Keywords**

Driving cycles, driving style, traffic conditions, electric vehicles, range estimation
Conventional and Unconventional Sintering of Alumina Ceramics with Addition of Waste Ceramic Powder

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**Introduction**  
Alumina ceramics are interesting materials for researchers due to their excellent properties like high hardness, thermal and chemical stability, which are controlled by the microstructure. Many attempts have been done to refine the microstructure by changing the composition and processing, like the densification of ceramic materials by sintering parameters control, which is an effective, simple and economical method. Recently, several unconventional sintering processes are studied for the production of high density ceramics.

**Aims**  
The aims of this study are: (i) obtaining of monolithic (Al₂O₃) ceramics without and with the addition of waste ceramic powder, (ii) shaping of alumina suspensions via slip casting, (iii) sintering of green bodies by conventional and unconventional methods and (iv) analyzing and comparing the properties of the obtained materials. For conventional sintering an electric furnace will be used to control the sintering process parameters. For unconventional sintering, two-stage sintering, microwave sintering and spark plasma sintering will be used. By achieving the above aims the development of a new material by recycling waste ceramic powder would influence the preservation of raw materials, reduce the amounts of deposited waste, and lower the production costs of monolithic alumina ceramic products.

**Methods**  
(i) Starting materials will be alumina powders (commercial and waste), and adequate additives, dispersants and binders will be selected. Analysis of commercial Al₂O₃ powder and waste Al₂O₃ powder will be done by XRD, ICP-OES, DSC, TGA, SEM, FTIR / Raman. (ii) Stable high-concentrated suspensions from commercial Al₂O₃ powder and waste powder will be prepared using different types and different amounts of additives, dispersants and binders. (iii) The suspension stability will be tested by the following parameters: rheological properties, zeta potential and the sedimentation tests. The optimal composition of a stable suspension for casting will be chosen. (iv) The green bodies will be shaped by slip casting into previously prepared plaster molds. (v) The green bodies will be characterized via density and microstructure-SEM-EDS analysis. (vi) The conventional one-stage sintering process and three unconventional processes will be compared: two-stage sintering, spark plasma sintering, and microwave sintering. The optimum sintering parameters (time, heating rate, temperature) will be selected using the design of experiments, specifically the response surface methodology to achieve the density as close to the theoretical density as possible. (vii) Analysis of sintered samples will include: the density by the Archimedes principle, the shrinkage after sintering, mass loss (using TGA method), samples morphology (microstructure and porosity) and mechanical properties (hardness and toughness).

**Expected scientific contribution**  
The expected scientific contribution of this study is the development of new materials based on monolithic alumina (Al₂O₃) ceramics with the addition of waste alumina powder, shaped via direct casting and with green bodies sintered by conventional and unconventional techniques: two-stage sintering, microwave sintering and spark plasma sintering will be applied.

**Acknowledgments**  
This work has been fully supported by Croatian Science Foundation under the project IP-2016-06-6000: Monolithic and Composite Advanced Ceramics for Wear and Corrosion Protection (WECOR).

**Keywords**  
Recycling, alumina ceramics, waste, microwave sintering, spark plasma sintering
Smart Factory Based on Lean Management Principles

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Introduction
The Fourth Industrial Revolution or Industry 4.0 creates factories of future or Smart factories. In a Smart factory cybernetic-physical systems control physical processes, they create a virtual copy of the physical world and make decentralized decisions. Through the Internet, these systems communicate and collaborate with each other and with people in real-time. Real world connects with virtual world. The aim of this paper is to develop a model of a Smart factory adapted to the conditions in Croatia and through the improvement of production and logistics processes to increase the efficiency of our companies and thus reduce their lagging for competition in Europe and the world. In order to ensure the maximum efficiency of the process, the Lean methodology will be applied.

Aims
It is mentioned that the main aim of the dissertation is to make a Croatian model of a Smart factory. Along with that, current state of Croatian companies regarding the readiness for implementing smart technology that is required by the Smart Factory will be described. Furthermore, metric will be defined, process monitoring system will be developed for all processes in a Smart factory model and the gap between domestic and foreign companies will be reduced.

Methods
After a detailed study of literature describing concepts of Smart factories, visits to fairs offering solutions in Industry 4.0 and smart technology, studying the Lean methodology and working on applying this methodology in companies, the next phase was made, which is the analysis of the current state of production enterprises in Croatia. The analysis came from a survey that filled enough Croatian companies in order to make a good conclusion. The results showed the readiness of companies for Industry 4.0. Further research continued to explore the prerequisites that are necessary to help companies to prepare for Industry 4.0. Further development of a smart business model is based on requirements of industry 4.0 and the use of modern computer-communication technologies (ICTs). A special part of this phase of the research will address how to set production and logistics processes and monitor their efficiency. In the next phase, smart factory model will be tested on two manufacturing companies. In the final phase, a smart factory model and selected concepts will be generalized.

Expected scientific contribution
The main scientific contribution is reflected in setting up an original smart factory model based on Lean principles.

Acknowledgments
PhD research will be financed by company Culmena.

Keywords
Industry 4.0, Smart factory, process approach to enterprise, lean management, logistics.
Numerical and Experimental Study of a Polymer Solar Thermal Collector

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Introduction
Nowadays, commercially available solar thermal collectors for domestic hot water preparation have reached high values of thermal efficiency. Although high thermal efficiency is achieved, their application is quite low, especially in Croatia. The main reason for that is a relatively high price. The need for an optimal combination of thermal, optical and mechanical properties limited the choice of materials that can potentially be used. Most common materials used are copper, steel, aluminum, and glass. Except for higher production costs, use of these materials does not allow easy design modification to improve thermal efficiency. Hence, the development of solar thermal technology is increasingly directed at the application of cheaper and more adaptable materials, such as polymers.

Aims
This research is focused on the development of a polymer solar collector considering the problem of material degradation while retaining or improving the thermal efficiency. The aim of the proposed research is to combine analytical and numerical calculations together with the experiment to develop a simulation model of heat transfer process in the polymer collector. Based on the model, optimal collector geometry will be recommended (as high as possible thermal efficiency under the predetermined conditions). Furthermore, this study investigates the impact of a newly designed collector on the entire system (thermal solar system with a tank or heat pump system) and analyzes quality measurement to determine its usability.

Methods
Heat transfer phenomena in the commercially available and polymer solar collectors are analyzed based on the literature survey and performed analytical and numerical simulations. Developed numerical models are validated via experimental testing on simplified solar collector assemblies. Based on the obtained data (heat flux and temperatures) and available polymer material properties, prototype design is proposed.

Expected scientific contribution
The expected scientific contribution of this research is following:
- the development of numerical models for the analysis of the heat transfer phenomena inside polymer solar thermal collectors with complex geometry
- a prototype of the newly designed low-price polymer solar collector
- determination of prototype usability via short and long-term laboratory thermal performance testing followed by the quality tests

Keywords
solar energy, polymer solar collectors, thermal efficiency, numerical models, measurements
Optimal Control for Plug-In Hybrid Electrical Vehicle with Parallel P2 Configuration

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Introduction
Goals of this research are aligned with the increasing need for transport electrification in order to reduce harmful greenhouse gas emissions. According to the statistical data, ¼ of the harmful greenhouse gas emissions in EU is caused by transport industry. Electrification of the transportation system will make vehicles more efficient, cleaner, quieter and reduce their dependence on fossil fuels. Electric vehicles are undoubtedly the future of green transportation but plug-in hybrid electrical vehicles (PHEV) are acceptable intermediate solution and it their market share is expected to grow. Although PHEVs are present on the market for some time now and contribute to the fuel consumption reduction, there is potential for further improvements through more efficient powertrain control for wide range of driving cycles.

Aims
New energy management control strategy for PHEV with parallel P2 configuration will be proposed with the aim to reduce fuel consumption for wide range of driving cycles. For this purpose, new optimal and integrated transmission gear shift control approach will be developed. The synthesis of the PHEV management system will be implemented for a wide range of changes in the road grade with emphasis on blended regime, and an adaptive driving strategy will be proposed based on categorization driving cycles in real time.

Methods
PHEV control variables optimisation, with the aim of minimising fuel consumption for a given driving cycle, is performed by the dynamic programming algorithm using the backward static vehicle model. Based on the insights gained from the optimisation, a synthesis of the energy management strategy for real-time application will be implemented. The backward vehicle model will also be used to evaluate the management strategy with regard to the globally optimal results obtained by DP optimisation. Forward dynamic vehicle model, which more accurately describes the dynamic behaviour of a vehicle, will be used for a more realistic vehicle simulation and fuel consumption analysis. Multi-criteria optimization using genetic algorithms will be used to create static maps for changing the transmission ratio. Energy management strategy parameters can also be optimised for various characteristic driving cycles to create rules for adapting the management system.

Expected scientific contribution
PHEVs with parallel configurations are relatively new innovation and they pose number of challenges to optimal energy management strategies that are not sufficiently explored in the literature. The challenges that are tackled in this research concern the control strategy of automatic Double Clutch Transmission (DCT) transmission in the parallel P2 configuration, the synthesis of the optimal management strategy for the case of pronounced changes in the road inclination (especially in the form of optimal trajectory of SoC in blended regime), and the synthesis of the adaptive energy management strategy with regards to driving cycle characteristics.

Keywords
Plug-in hybrid electirc vehicle(PHEV), energy management control strategy, optimal control, P2 parallel configuration
**Preparation and Characterization of Advanced Photocatalysts**

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**Introduction**

Environmental pollution and the destruction of the environment is a very serious problem faced by today's people. A major problem in environment is water and water flows protection. Science has tried to solve this problem for a long time been involved, and scientists are constantly trying to innovate and improve methods to raise levels of water purification to new levels. The appearance of micro-polluting substances in the purified sewage and drinking water influenced the scientific community to direct their work towards finding a solution for removing micro-pollutants from the water. Micro-pollutants include human and veterinary medicines, chemicals from the industry, pesticides which, due to the continuous production processes, are constantly recirculating in the environment, mainly because of production processes, or by disposing of unused or obsolete products. At the moment, two processes of water purification from micro-pollutants, adsorption on activated carbon and ozone are used at the industry level. Given the complexity of these methods, scientists are working on finding cheaper solutions, one of which could be an advanced oxidation process, such as photocatalysis where complete degradation of contamination (mineralization) occurs and is characterized by the emergence of completely non-hazardous degradation products.

**Aims**

The aim of this assignment would be to develop a stable TiO₂ immobilized photocatalyst with a long-term efficacy on glass meshes that can be used as a carrier. It is necessary to establish a precise process of preparation by firstly finding a similar method in the literature and then, by the method of attempts and errors of changing the process parameters such as TiO₂ mass, suspension concentration, mixing time, temperature, drying and application layer to determine the best application method. Determined methodology will be used to perform binding of TiO₂ to the carrier. Testing for the stability of the TiO₂ and durability of the catalyst will be carried out through photocatalytic experiments such as the degradation of salicylic acid as a modal organic pollutant.

**Methods**

For the purpose of the development of photocatalysis with the immobilized TiO₂, the sol-gel method for the TiO₂ application to glass fiber meshes will be used. In order to confirm the presence and the stability of the TiO₂ particles, the surface morphology of glass meshes before and after immobilization by scanning electron microscope (SEM) and chemical composition by energy-dissipative X-ray spectroscopy (EDS) will be analyzed. Determination of the photocatalytic activity of immobilized TiO₂ will be investigated in the pilot reactor on modal water solution through degradation of salicylic acid. Reaction of degradation will be monitored by the UV-VIS spectrophotometer.

**Expected scientific contribution**

The expected scientific contribution is to find and develop the best possible TiO₂ immobilization method on glass meshes for use in advanced oxidation process, photocatalysis in order to purify waste water from micro pollutants.

**Keywords**

Titanium dioxide, immobilization, sol-gel, photocatalysis
Thermodynamics of Metallurgical Processes of Advanced Metallic Materials

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Introduction
Tool steels belongs to the category of advanced metal materials, and are used primarily in the manufacturing of various types of tools. They are subjected to various compression and wear processes, so the maximum durability and the minimal maintenance is required. The most common application of tool steels is in different kinds of industrial plants, such as: thermal machines and devices, chemical and process industry equipment, thermal and nuclear power plants, metal and ceramic forming tools intended for operation at elevated and high temperatures. Therefore, tool steels must possess special properties, such as: increased hardness and wear resistance, strength durability at increased temperatures, good behaviour of the material when during heat treatment, corrosion resistance etc.

Aims
This research paper shall cover a group of tool steels intended for operation in the hot state. In order to achieve properties such as: an elevated hardness and wear resistance, strength durability at elevated temperatures, thermal machinability etc., it is important to select an adequate chemical composition of the material. The afore-mentioned material properties can be achieved by alloying, i.e. by adding elements which would enable the formation of carbides to at increasie the wear resistance, as well as the resistance to loosening. Achieving good properties is enabled by alloying with chromium, tungsten, vanadium, molybdenum or cobalt. In doing so, it is very important to know the precise quantity of added alloying elements and to be familiar with the production process, because the formed compounds change during the production process, and influence to the transformation processes.

Methods
Part of the research would include the design of chemical composition, calculations and thermodynamic parameters of the equilibrium phase diagram. One of the experimental methods by which the mentioned parameters can be achieved is the use of thermodynamic programs such as Thermo-Calc. This method would provide certain thermodynamic parameters that are suitable for describing the system and predicting the phase diagrams. The main objective of the survey is to determine an adequate chemical composition for achieving the required properties, while still enabling the resistance of the product to corrosion which occurs in the environment where the product is used. Therefore, a part of the survey would be focused on examining possibilities of the occurence of corrosion processes and the investigation of corrosion resistance of the material in a corrosive medium.

Expected scientific contribution
Modern industrial development would be almost impossible without such types of material. Therefore, new implementations and improvements of the specific material properties are very important in motivation for further research of tool steels. This particularly concerns the tool steels used in operation in the hot state for which the areas of temperature stability of a specific phase could be monitored, as well as the change in the concentration of a specific phase.

Acknowledgments
This investigation has been performed in the frame of financial support of investigation of University of Zagreb (TP167 Design and characterization of innovative engineering alloys) and collaboration between University of Zagreb Faculty of Metallurgy a

Keywords
Tool steels, metallurgical processes, thermodynamics, alloying elements
The Effect of Vibration on Orthodontic Tooth Movement

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Introduction
Dental biomechanics has so far been studied at several levels but the results of these studies still do not give a complete picture of tooth movement and alveolar bone remodeling. In the jaw, on the pressure side, the bone is resorbed while on the tensile side bone mineralization occurs resulting in the formation of new bone. The orthodontic tooth movement (OTM) is the result of orthodontic and chewing forces and mechanically excited biological processes. OTM does not necessarily occur immediately after application of force. The static orthodontic force causes small initial movements immediately after application, however, only after some time the tooth moves to the predetermined targeted position. Today’s technology is not sufficient for direct, in vivo measurements of mechanical properties of periodontal ligament (PDL), due to the geometry of PDL, a very thin structure, which makes modeling of this complicated structure very difficult. Numerous studies that have been carried out were focused mainly on the effects of static orthodontic force on teeth and, in addition to the clinical studies carried out, numerical models that predict tooth movement within a certain time frame have been developed. In the jaw, in addition to the static orthodontic force, there are also dynamic forces, such as chewing forces, contact forces with soft tissue, and occlusion forces. Only very recent studies have begun focusing on the impact of dynamic load on bone remodeling during OTM, and future research needs to include the influence of dynamic forces on tooth movements to understand what is happening during this process.

Aims
The aim of this research is to develop a numerical model that will describe bone remodeling in the alveolar bone by simultaneously applying static orthodontic force and cyclic loading (vibration).

Methods
The research will be carried out on the upper single-rooted teeth. A numerical model describing the remodeling of the alveolar bone during orthodontic treatment will be developed. The model will include teeth, periodontal ligament and alveolar bone (cortical and cancellous bone). The model will be patient specific and in order to obtain teeth geometry, software Materialise Mimics and 3-matic will be used. The model will describe the displacement of the teeth that is the result of a simultaneous action of a static orthodontic force and dynamic loads. The model will be implemented into the finite element method software, Abaqus, for discretization and numerical simulation of orthodontic teeth movement with parameters obtained from clinical practice. Validation of results will be performed by comparing experimental data from the literature.

Expected scientific contribution
Novel numerical model of single-rooted teeth that describe OTM could be developed. The model could confirm the effect of vibration on accelerating the process. Such a model could be a useful tool for orthodontists as it would predict a time frame of OTM.

Acknowledgments
The research will be funded from the support of the University of Zagreb and RN02407 (project managed by Tanja Jurčević-Lulić, Ph.D.). Micro CT recordings will be provided, free of charge, by the Dental Polyclinic of Apolonia, Zagreb.

Keywords
orthodontic tooth movement, alveolar bone remodeling, biomechanical numerical model, periodontal ligament, cyclic load
Effect of Mass Unbalance and Thrust Force Asymmetry on Dispersion of Unguided Reactive Projectiles

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Introduction
Production of ammunition is a process characterized by high demands on manufacturers, with tolerances set more strict than would be acceptable for civilian production. Insisting on such high quality is understandable, because modern artillery is shooting at distances of 30 km or more, while the expected error still must be kept under one hundred meters (even for unguided ammo). Any asymmetry will significantly increase dispersion of hits.

Aims
The aim of this research is to create a nondeterministic model of missile flight with six degrees of freedom (6DOF) that will show the trajectory sensitivity to various disturbances. The model will be applied to the selected unguided reactive missile and will include the impact of mass imbalance and of reactive force asymmetry as stochastic disturbances. Using such developed model it will be possible to assess correlation between a specific disturbance and a final dispersion of hit points, as well the impact of particular disturbance on missile stability.

Methods
After an overview and detailed analysis of literature, a detailed CAD model of the missile will be prepared. All missiles’ characteristics of interest will be also gathered or evaluated, e.g. aerodynamic coefficients as function of Mach number, reactive force during active phase and missile’s inertial characteristics. Since the mass distribution is of special interest in this work, the model of missile will be created assuring that later realistic causes of mass asymmetry could be introduced.

As for the model of missile trajectory there will be prepared a 6DOF model, suitable both for classical artillery projectiles as well as for reactive missiles. This model will allow us to include main before mentioned disturbances during the flight. Parameters having the most impact on missile flight are related to weapon or the launch system, then to atmospheric condition and finally to imperfection of missile itself.

A Monte-Carlo simulation will be carried out, introducing possible imperfections and generally variations of main influential parameters. An example would be a distribution of mass that generally will not be symmetrical with regard to outer profile’s axes of symmetry, causing static and dynamic asymmetry. Principal axes of inertia will not coincide with outer profile’s axes of symmetry.

Expected scientific contribution
A clear two-way correlation will be obtained: on one side to help estimate boundaries of hit points dispersion based on expected disturbances, and on the other side to show allowed asymmetries (as guidance to manufacturers) in order to achieve previously determined boundaries of dispersion.

Also it will be shown that traditionally used test or criteria to determine if the projectile production meets necessary standards is not sufficient to guarantee that dispersion will remain in narrow boundaries.

Acknowledgments
This work is supported by the MoD of the Republic of Croatia.

Keywords
6DOF, mass asymmetry, asymmetry of reactive force, dispersion
Analysing Team Activities in Engineering Design

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**Introduction**  
To increase the potential of solving design problems, critical tasks in design are often conducted as team activities (e.g. idea-generation, concept selection etc.). Teamwork is useful in design as it facilitates the exchange of ideas, knowledge and resources, and thus affects the outputs of the design process (ideas, decisions etc.). To better understand both the design process and teamwork, researchers often study team activities. These studies are usually grounded on the work from other fields, such as psychology, sociology, neuroscience etc. Even the most common method for studying designers, protocol analysis, is taken from psychology. Since research efforts of studying design process from the designer’s perspective are relatively recent, there is still lack of models to describe team activities and methods for analysing design teams. These models and methods should help in exploring the concept of the design process as a human act. However, although teamwork has been the subject of design research for the last 40 years, researchers still point out the lack of unified methods to study design teams.

**Aims**  
This work aims to develop models for describing the team activities and methods for analysing teamwork in design. The models will cover various teamwork features, such as the inputs (individual characteristics, team size, type of design task etc.), the process (communication, interaction etc.), and the outputs (e.g. concept, product etc.). Methods will aim to combine the proposed models thus giving the possibility to conduct a more comprehensive analysis of teamwork.

**Methods**  
The research will be based on the elements of the Design Research Methodology. Firstly, a literature review and initial set of experiments will form a basic understanding of existing models and factors which influence teamwork. Based on these insights, models will be developed to cover various teamwork features. Then, the models will be combined, and methods for analysing teamwork will be proposed. Models and methods will then be theoretically and empirically validated using the Validation Square framework.

**Expected scientific contribution**  
The proposed research is expected to have the contribution for both, design theory and design practice. Theoretical contribution manifests in the models and methods for analysing teamwork which would aid researchers in understanding teamwork in design and the design process. The contribution to practice is in the development of tools for analysing teamwork which can be used by project managers to observe teams and identify potential problems.

**Acknowledgments**  
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**Keywords**  
teamwork, engineering design teams, protocol analysis
Numerical Modeling of Piezoelectric Materials

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Introduction
Prediction of failure in brittle materials is an interesting topic of research, thus many numerical models incorporating continuum theories have been developed. In numerical models based on continuum theories, complicated procedures in describing phenomena depending on lower scales (e.g. microscale), like capturing the finite size of fracture process zone, modeling multiple cracks, fragmenting, etc., are needed. An interesting and valuable alternative to this models are lattice models, where a solid is represented as an assembly of simple beam finite elements representing cohesion forces between rigid particles inside the material. Since typical piezoelectric materials are brittle (e.g. PZT ceramics), the idea is to use lattice models in modeling of failure in piezoelectric materials, where coupled electromechanical constitutive model in finite element modeling is needed. The main idea is development of the numerical model capable of the failure modeling in other areas of multiphysics.

Aims
The first aim of the research is the development of the piezoelectric truss element and its implementation in the lattice model. After piezoelectric truss element, piezoelectric beam element based on Timoshenko theory can be made and implemented in the lattice model. When this is accomplished, the model will be extended to analyze damage and failure of the piezoelectric materials.

Methods
Discretization of the domain can be regular, with equal hexagonal or square unit cells and all elements have the same properties (length, cross-section, moment of inertia, Young’s modulus, etc.), or irregular, with discretization of the domain based on Voronoi tessellation, with edges of Delaunay triangles as lattice elements. While irregular lattices cannot represent the uniform straining of a solid exactly, they are better suited for capturing the direction of crack propagation correctly and to describe the material heterogeneity at lower scales. Lattice elements used in this analysis will be beam finite elements based on Timoshenko theory, with two displacements, one rotation and electric potential as degrees of freedom in each node.

Software FEAP with subroutines written in Fortran will be used for finite element analysis.

Expected scientific contribution
Lattice models are developed only for materials in which strain depends only on mechanical loading. For piezoelectric materials, there are only continuum finite elements developed. The developed piezoelectric lattice model will be proposed for the first time in order to offer an alternative discrete approach that should be applicable at lower scales for better insight into the fracture process of piezoelectric materials.

Keywords
piezoelectric materials, finite element method, lattice model, Timoshenko beam finite element
Influence of Shielding Gas Composition on Microstructure and Mechanical Properties of Wire and ARC Additive Manufactured Inconel 625

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**Introduction**  
Wire and Arc Additive Manufacturing (WAAM) is relatively new and rapidly advancing technology for manufacturing large and complex geometry components. It is particularly important for expensive materials such as nickel-based superalloys due to very low material waste and thus significant cost savings. Inconel 625 is the most common nickel-based superalloy used for diverse industry applications. It is characterized by an attractive combination of high tensile and fatigue strength and excellent corrosion resistance in aggressive environments. Furthermore, Inconel 625 has a great weldability when is welded by conventional Gas Metal Arc Welding (GMAW) process, making it suitable material for WAAM.

**Aims**  
Shielding gas used for protecting molten pool during metal deposition is one of the key WAAM process parameters. It has a great impact on microstructure and mechanical properties of wire and arc additively manufactured component as well as the large influence on the other welding parameters. Firstly, the aim of this research is determination of optimal welding technology to obtain stable process. Secondly, investigation of the microstructure and the mechanical properties of samples manufactured by using different shielding gas mixtures and welding parameters is the main aim of the research.

**Methods**  
In the first part of research combination of theoretical research and preliminary experiments will be used to obtain optimal welding technology for different sets of process parameters. Once the parameters has been set several samples will be manufactured. Subsequently, a number of non-destructive and destructive tests will be conducted upon the samples. Finally, data will be analysed and the influence of the input variables will be evaluated.

**Expected scientific contribution**  
The research will significantly contribute to the understanding of the WAAM process parameters influence on mechanical properties of manufactured components. Furthermore, usability of wire and arc additively manufactured nickel alloy components will be assessed. Results will significantly play a part in the development and application of wire and arc added manufacturing.

**Keywords**  
WAAM, Inconel 625, GMAW
Numerical Modelling of the Co-Firing of Pulverised Coal and Non-Conventional Solid Fuels

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Introduction
For a reliable numerical calculation of co-firing of solid fuels, there are several mechanisms that have to be modelled accurately. For this purpose Euler/Langrangian framework was used to investigate flow pattern and combustion process of coal and biomass blend. This implies simulation of turbulent, reacting flow with all three heat transfer mechanisms, where reacting flow includes particle drying, pyrolysis and char and volatile oxidation. The focus of this work is to develop a method for numerical calculation of the co-firing of pulverised coal and the biomass under various fuel blending ratios. In this work, effects of biomass particle size and shape on residence time will be investigated, which is also prerequisite for the accurate pollutant emission estimation. Additionally, along with the emission and absorption of the participating triatomic gases, absorption and scattering of thermal radiation by solid fuel and flying ash particles have to be modelled. In the experimental part of the research, relevant physical quantities will be measured on the lab-scale furnace within Faculty of Mechanical Engineering, University of Sarajevo. Finally, developed method will be evaluated by comparing results obtained by the numerical calculation with the results derived from experimental measurements.

Aims
The main goal of this research is to develop a numerical method that is capable of simulating co-firing processes of the pulverised coal and the biomass using Euler/Lagrangian approach. Outcome of this work will give more accurate pollutant emission estimations, especially NOx, whose reduction is a major advantage of this technology. As a prerequisite for that, it is necessary to model all heat and mass transfer mechanisms between continuous and solid phase. Also, it is necessary to model in detail particle drying, pyrolysis and char and volatile oxidation processes to investigate how it affects the flow pattern and the flame structure. Main goal of this research is to develop such model that would confirm the hypothesis by comparing the simulation results with the results obtained by the experimental measurements.

Methods
This research is performed using finite volume method approach. Fluid flow and heat and mass transfer between continuous and discrete phase are described using Euler/Lagrangian approach. In the end, results obtained by the numerical calculations were compared to the available validation data.

Expected scientific contribution
The outcome of this work is numerical method that would enable computation of turbulent, reactive flow with the heat transfer during the process of co-firing of pulverised coal and biomass. It will show how application of the Euler/Lagrangian approach for modeling of co-firing process with detailed kinetic mechanisms, results with better understanding of phenomena that occurs in the furnaces where coal and pulverized biomass are burned.

Keywords
chemical reactions, combustion, radiation, heat transfer, solid particles
Modelling Fluid-Structure Interaction for a Micro Aerial Vehicle

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Introduction
Unmanned aerial vehicles (UAVs) have already become a standard tool for a wide range of applications. Both quadrotor and fixed-wing configurations of UAVs are available on the market and both configurations are already in commercial use. Quadrotor UAVs are popular for their hovering capabilities, vertical take-off and landing (VTOL), affordability and great maneuverability. However, these advantages come at a price of low efficiency and high noise. On the other hand, fixed-wing aircrafts lack hovering and VTOL capabilities, but have much better efficiency. However, both configurations don’t scale well to small sizes. In short, there is no available flying configuration that satisfies requirements on small size, low noise, high energy efficiency, high maneuverability and VTOL. Therefore, researchers have recently focused on nature to seek solutions to the problem of flying at small size. The intuition is to focus on insects, since they are able to accomplish all these requirements. They accomplish this by flapping their wings at high frequencies with complex wing motion, creating vortices at both leading and trailing edge of the wing, and using those vortices for lift and propulsion. However, as soon as it was discovered how insects fly, it was obvious that it will be a difficult task to design a manmade object that will mimic this behavior. One of the main difficulties is understanding all important aerodynamic phenomena that insects use for flying, and first step to better understanding is better computational model of the insect-fluid system.

Aims
The aim of this work is to develop a better fluid-structure interaction (FSI) model for a flapping wing micro aerial vehicle, that is capable of modeling all important phenomena, at numerical cost that allows for usage of the model both in design optimization loop and optimal control.

Methods
The main tool for developing an efficient FSI model are fluid reductions arising from geometry mechanics. By using these reductions, it is possible to develop a monolithic solver, since the fluid is described only by the additional inertia added to the solid variables. The reduced FSI model will be supplemented with the mechanisms for describing vorticity effects.

Expected scientific contribution
The expected scientific contribution is the novel efficient FSI model for flapping wing micro aerial vehicle. The model will simulate fluid effects by integrating only over a boundary of the solid, using efficient implementation of boundary element method, avoiding spatial discretization of the fluid domain. This model is expected to be efficient and accurate enough to allow for usage in both design optimization loop and optimal control.

Acknowledgment
This work has been supported in part by Croatian Science Foundation under the project IP-2016-06-6696.

Keywords
Fluid-structure interaction, Unmanned aerial vehicles, Geometric reduction, Efficient simulation
Introduction
Liquefied natural gas (LNG) market is continuously growing, and nowadays LNG is more and more used as a ship fuel. As a consequence of market growth, ever larger LNG ships, as a key part of transportation chain, are being built. Besides strategic importance of LNG for the country its importance is obvious bearing in mind that it requires relatively large number of highly qualified experts. The fact that only several countries in the world have developed LNG transportation technology confirms complexity of LNG industry. Also, it is not realistic to expect that energy needs of large merchant ships can be fully covered from renewables in the near future. Therefore, having in mind low-carbon strategy of EU expansion of LNG network is of high importance.

Most of the existing LNG fleets use diesel engines driven by diesel fuel and mechanical propulsion chain. There are several advantages of LNG as a ship fuel over heavy fuel oil (HFO), particularly in the Emission Control Areas (ECAs), but it is still not used as it could be, particularly due to underdeveloped infrastructure worldwide. The marine power system development trend is developing integrated power systems, offering greater energy efficiency, and using liquid natural gas as fuel for prime movers environmental eligibility.

Aims
The aim of the research is investigate and analyse the trends in building of LNG ships, with particular emphasis to their cargo containment systems and powering characteristics, having in mind above mentioned facts on LNG as a ship fuel and develop procedures for design high degree energy efficient and environmental eligible power system of the LNG ships using LNG as propulsion fuel.

Methods
The database IHF Fairplay, that represents the World Register of Ships (IHS WROS), and includes data on all merchant ships and newbuilding orders at that time, will be used to analyse trends in building of LNG ships. Also, analysis of the power systems of the existing LNG fleet will be carried out as well as an analysis of the influencing factors on the parameters for assessing energy efficiency and environmental eligibility. The performance of marine power system of ships that have already been built will be evaluated, according to different criteria, and alternative solutions that meet rigorous environmental rules will be offered. At the end, assessment of the impact of the LNG ships fleet on the environment depending on the different configurations of marine power systems will be done.

Expected scientific contribution
The obtained results are useful for ship owners, ship designers, classification societies and other regulatory institutions, as well as for all other parties involved in LNG business. That results is related to challenges, basic principles and solutions in building of LNG ships. Also is related to elaborated designing procedures of a high degree energy efficiency and environment acceptability marine power systems of LNG ships. Designing procedures will be elaborated through the impact analysis of the various configurations of the marine power systems on the energy and environmental ship features taking into account not only the design but also the operational features of the ship.

Keywords
sea transportation, LNG ship, liquefied natural gas, ship power system
Technical and Economic Potential of Seawater Heat Pump with Storage Tank Integrated into a Hotel Located on the Mediterranean Coast

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**Introduction**  
The heat pumps are recognized as energy efficient and environmentally friendly technologies for cooling and heating. Due to ability to convert electrical energy to heating and cooling energy, which can then be stored in thermal tanks, their greatest potential can be found in pairing them with smart grid systems. By pairing, heat pumps can contribute in making the power grid more dynamic, but also in reducing electricity costs for heating and cooling.

**Aims**  
The objective of this work is to identify the technical and economic potential of using heat pumps with thermal storage tanks in hotels located on the Mediterranean coast.

**Methods**  
Energy demand was studied for a complete year on an hourly basis, and an economic analysis was made for the best choice of storage capacity. For the economic analysis, as well as storage analysis, the electricity prices on energy demand market were used. Days with the highest, lowest and average demands in both heating and cooling season were taken as representative days, with which the possibilities to regulate expansions were presented.

**Expected scientific contribution**  
Lately, heat pumps with thermal storage thanks have been widely researched, but mostly for the heating regime. This work analyses the use of heat pumps with storage tanks for cooling regime. When proven that heat pumps with storage tanks are a cost-effective technology for regarded hotel, it will be possible to further analyse the impact of installing heat pumps in all the hotels at Mediterranean coast and to study what impact that would have on the power grid.

**Keywords**  
Heat pumps, storage tanks, hotels
Assessment of the Technical Potential of Agricultural Residues and Biowaste for Bioenergy Use on the NUTS 3 Level

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Introduction
Bioenergy can be produced from a range of feedstocks and utilized for production of renewable electricity, thermal energy or transportation fuels. Using feedstocks that have been grown on agricultural land has caused concerns over the negative environmental impact due to indirect land use change. Consequently, feedstocks such as agricultural and industrial residues and by-products are receiving increasing policy support from the European Union.

Aims
The main objective of this work is to elaborate a method for assessment of the technical potential of available agricultural residues and biowaste for bioenergy production.

Methods
This method takes into account residues which occurs during agricultural production and human consumption. These stages were analysed for five sectors: fruits, vegetables, cereals, industrial crops, and animals. When estimating the potential of available residues, the residue-to-product ratios were used. In order to quantify the technical potential of mentioned feedstocks, their current use was subtracted from the total available amount. Spatial distribution was also taken into consideration, by calculating the technical potential of residues and by-products for the NUTS-3 regions.

Expected scientific contribution
There have been numerous studies and scientific papers which used the statistical method to assess the technical potential for different biomass residues (mostly for one which occurs during cereal and livestock production). However, most of these works are providing the results on the national level, what doesn’t give the insight to the spatial distribution of the technical potential. Assessing the potential on a smaller level (such as NUT 3 level) provides the identification of the regions with higher technical potential, which could be considered as the most suitable for installing bioenergy production entity.

Acknowledgments
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Keywords
bioenergy, technical potential, feedstocks, residues, by-products
Lean Toolbox – Back to Basics

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Introduction
Lean production (LP) was presented to Croatian industry more than five years ago. Many organisations have achieved great results through lean, but many of them failed to make desired goals due to lack of lean understanding and loss of enthusiasm.

Methods
This study was made on Croatian organisations that have tried to implement lean manufacturing. Nearly 300 organisations were interviewed, while 63 organisations were identified as lean users. Mentioned study was launched in order to capture best lean tools implementation framework for waste elimination.

Preliminary results
LP is used in Croatia mostly by medium and large companies, where manufacturing industry was lean pioneer and put major effort in lean concept acceptance. Lean is adopted correctly mostly by large Croatian companies, where market leaders are most successful in lean implementation. Main reasons for going lean in Croatia are connected with performance improvement desire and seen lean benefits. These triggers for going lean are far different than triggers documented on studies made on western companies. For example, study made in UK has revealed that main reason for going lean is connected with market pressure. However, aspirations or desired goals by going lean are pretty much the same in Croatia and UK. Mostly this aspirations are connected with increase of efficiency, profitability, productivity, elimination of waste, reduction of manufacturing cost etc. Study made on 63 Croatian companies revealed us next key elements: What type and scale of waste are most common for Croatian companies? Which lean tools are most frequently used? Which tools had most positive impact? What was the progress in reduction or even elimination of waste?. There are numerous lean tools, but tools considered in this survey were 25 basic lean tools. Most frequently used tools among Croatian industry are standardization of work, kaizen (continuous improvement), 5S, Key Performance Indicators (KPI), Value Stream Mapping (VSM), bottleneck analysis, SMART goals, visual factory, Just-In-Time (JIT), Muda (Waste), Single-Minute Exchange of Dies (SMED), Total Productive Maintenance (TPM) etc. Some lean tools were documented through this survey as tools with most positive impact. Therefore we can say that Kaizen, Standardised Work, Hoshin Kanri, Continuous Flow, Muda, Jidoka, Bottleneck Analysis, SMART Goals and Visual Factory have positive impact more than 90% among all participants of this study.

Discussion
Generally saying lean is philosophy, culture and way of living. However cultural changes have to be provoked by seen best practices. This survey documented best practices among most successful lean organisations and pinpointed lean transition key elements

Acknowledgments
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Keywords
lean tools, waste reduction, lean implementation
The Impact of District Cooling Systems on the Integration of Renewable Energy Sources in Arid Climates

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Introduction
District cooling has become a widespread cooling technology in a region like Dubai with hot-humid climates. Currently all cooling system operation in Dubai is based on vapor compression refrigeration systems with a 100% conventional power supply. The goal is to examine the impact of district cooling systems on the integration of renewable energy sources into future energy systems from the perspective of energy planning.

Methods
The approach is based on a combination of absorption chillers, vapor compression chillers and thermal storage tanks resulting in effective system than using a single type of cooling technology. Power mapping, conventional mapping, district cooling mapping and renewable energy mapping of Dubai cooling demands and the existing district cooling facilities, capacity and way of usage and the expecting future consumption growth are certain steps used for this work. Following the energy mapping, several energy system model will be developed in EnergyPLAN and the mapping shall be conducted from year 2017 up to 2050 with three milestones, each stage (2017, 2030 and 2050) Two scenarios will be used in this work, namely Scenario 1: both the vapor compression and the absorption cooling systems work together during the day and vapor compression works during the night. For Scenario 2: 10% reduction in the cooling capacity of the vapor compression to save power. 50% of the vapor compression that works during the night and 40% of the absorption cooling system along with 10% of the cold storage tank work together during the day.

Preliminary results
The integration of renewable energy sources and district cooling with the power sector will result in a decrease in the critical excess electricity production.

Discussion
The scientific contribution of this research work will be the quantification of the impact that district cooling has on the integration of intermittent renewable energy sources in the overall energy systems in hot and arid climates, the environmental and economic analysis of the integration of district cooling systems & renewable energy sources and also a new cooling scheme for arid climates based on the combination of vapour compression, absorption cooling and thermal storage. Thermal storage tanks are used to improve chiller plant efficiency and to optimize the use of electrical power by saving the electrical peak demands. Solar district cooling benefits energy saving and energy planning through two aspects: its eco-friendly features and district cooling systems are 25%-50% more energy efficient. The hypothesis of these research is that district cooling systems (absorption / vapor compression / thermal storage tanks combination) in hot and arid climates coupled with the power system can increase the economically feasible level of penetration of variable renewable energy sources, primarily solar, and reduce greenhouse gas emission.

Keywords
Solar-powered photovoltaic (PV) panels, Renewable energy, Absorption chillers, Thermal storage tanks, Energy-PLAN
Risk-Based Decision Support System for
Ship Manoeuvring in Rough Seas

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Introduction
Weather forecasts and experience of the seafarers help them to avoid rough sea and consequently problems with structure, cargo and safety. Sometimes is impossible to avoid rough sea because of the reasons such as small area of a sea, obligatory route separation etc. In that occasions ship manoeuvring such as speed and course corrections has crucial role. The aim of the research is to examine the possibility that the ship's officer in real time determines the optimal route at a rough sea, due to the seakeeping and safety requirements, using relatively fast and accessible mathematical calculations. As a criterion for decision-making, it will be proposed to minimize total risk, according to the criteria of operability that were determined by conducting a specially designed survey among experienced seafarers.

Methods
Survey among experienced seafarers was made on Faculty of maritime Studies in Split in way to determine interesting rough sea operability criteria for ships. It was done with specially prepared questionnaire and conversation with seafarers. Results of the survey are being currently analyzed.

Ship motion data were collected from different ships in the Adriatic and North Sea with inertial sensors, both professional and self-made devices. This survey was done by author during 2016 and 2017. Various sea state conditions and different ship headings were included.

Both, numerical and semi-analytical ship motions calculations were made and compared to the collected data from the real ships.

All mentioned methods and actions are fundamentals for risk calculations and sailing routes optimization that will be done. Determined operational criteria from seafarers’ questionnaires will be included in risk calculations. Possible routes in storms (rough sea) will be optimized with base in ship manoeuvring and risk calculations.

Decision making algorithm, accessible to all seafarers, will be result of the research

Preliminary results
Result of the questionnaire and conversations among seafarers are new and improved operational criteria.

Numerical and semi-analytical ship motion calculations were improved and validated with collected motions data from the real ships.

Discussion
Risk calculations and sailing route optimizations have to be done and final result, decision making algorithm, has to be tested in real life. During previous work some uncertainties have been noticed. Mathematical expression of operability criteria in ship manoeuvring described by seafarers in the questionnaires will be challenge for the author. Finally, real life testing of the result-decision making algorithm will be real challenge of the total research.

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Scientific project HRZZ 8722 GASDORP

Keywords
ship sailing route, seakeeping, decision making
Low-Cycle Fatigue of Damaged Stiffened Panels and Damaged Ship Structure

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**Introduction**  
During safety assessment of a damaged ship hull it is generally considered that the damage is time invariant. However, the initial damage caused by collision or grounding can further propagate during the ship salvage operations, in a similar way as large fatigue cracks. This research aims to extend the conventional post-accidental structural safety assessment by investigating the possibility of damage propagation in damaged ship hull during salvage period as low-cycle high-stress fatigue process caused by fluctuating wave loads. Low-cycle loading can cause high-amplitude stresses at the edge of damage opening, which consequently lead to high stress concentrations and appearance of low-cycle fatigue (LCF). This could occur in a scenario where a damaged ship encounters a severe storm during the salvage period. Importance of the LCF is such that it should be considered as principal failure mode, associated with ultimate limit state (ULS) or accidental limit state (ALS).

**Methods**  
In this research for conceptual considerations, damage shape of damaged stiffened panel is idealized as rectangular, diamond and circular. A finite element (FE) model is created for intact stiffened panel in order to calculate the nominal stress, as well as for each idealized damage shape, for which the stress concentration factor is then calculated. The number of constant-amplitude wave load cycles to initiate a LCF damage propagation is calculated under the assumption of linear cumulative damage and the strain-life method, according to Det Norske Veritas classification notes. Accumulated LCF damage is then estimated by Monte Carlo simulation, with individual stress amplitudes drawn as random numbers according to Rayleigh distribution. The analysis is performed for three assumed types of short-term random sea state: calm, moderate and rough seas.

**Preliminary results**  
It was found that both the damage shape and severity of sea state have effect on LCF. For calm and moderate sea states LCF damage accumulation is negligible. For the case of the diamond shape damage, the results are much more significant and the accumulated LCF reads between 0.5 and 0.8. This shows that in some unfavorable circumstance such as rough sea and diamond shaped damage, LCF could occur at the damage tip and the damage could start propagating. In such case, the crack propagation across stiffened panels should be further analyzed.

**Discussion**  
The cyclic material properties and parameters in the strain-life equation vary in the literature. Some authors proposed calculating these parameters by assuming the dependency of various criteria on the Brinell hardness as the key parameter. Classification rules prescribe conservative design values of these parameters. It is necessary to make parametric analysis of input data in order to examine the effect of the parameters variation on the LCF. Further research will include implementation of previous method onto realistically damaged ship structure.

**Acknowledgments**  
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**Keywords**  
Low-cycle fatigue, Collision, Damage propagation, Fluctuating wave-loading, Stress intensity factor
Introduction
Learning from demonstration is a very progressive field in modern robotics. It shifts the problem of robot programming from low level code writing and point-to-point teaching to programming through intuitive interaction with the robot. This enables easier use of robots from the human operator position and brings a framework for faster implementation of robotic automation in industrial environments. The field of learning by demonstration ranges from imitating demonstrations on the trajectory level to composing task oriented plans from predefined movement primitives.

Methods
An approach that enables robots to imitate human-demonstrated trajectories in a task oriented way is proposed in this paper. Here, demonstrations are provided through human-robot kinesthetic and teleoperation teaching which eliminates the notion of the correspondence problem. A novel task parameter detection algorithm based on the Inverse reinforcement learning algorithm (IRL) is used for the clustering of useful task parameters from multiple observed demonstrations by a similarity criterion. These parameters are obtained in a raw form through an implemented visual tracking system covering the robot working space and recording demonstrations. Then motion characteristics of Dynamic movement primitives (DMP) are exploited to generate initial imitation based trajectories which are then further optimized through previously determined task parameters.

Preliminary results
In the execution phase, the approach provides task generalization when performing from different initial conditions and trajectories are enabled for collision avoidance by the introduction of an additional coupling term in the movement’s differential equation. The approach is evaluated on two-dimensional task constrained manipulation problems which include robot sweeping.

Discussion
The research presents a method for robot trajectory learning from human demonstration in a task oriented way. In general, robot movements have to be learned and performed in a continuous natural-like form. This can be guaranteed by modeling trajectories with models based on dynamical systems. Task execution can be incorporated in the model through the extraction of important task features which serve as objectives when generating a task based trajectory. The approach has the potential to be tested in learning and performing three-dimensional robotic tasks.

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Keywords
Robot learning, demonstration, movement primitives, task parameters
Numerical Modelling of the Effects of Biofouling on Ship Resistance and Propulsion Characteristics

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Introduction
Biofouling is the accumulation of microorganisms, plants, algae, or animals on wetted surfaces and it represents a growing problem from both economic and environmental point of view. Even though it occurs in many different fields, shipping industry is the most affected by the settlement and the growth of biofouling organisms. Ship hull roughness is increased because of presence of biofouling organisms and consequently, hydrodynamic performance of a ship is reduced, which results in increased fuel consumption, reduction of the ship speed and increased emission of harmful gases. Presently, there is no comprehensive procedure which could reliably predict the effect of biofouling on the ship hydrodynamic characteristics. The importance of the assessment of these effects was recognized by the International Towing Tank Conference (ITTC), which highlighted the importance of a development of a new formulae or methods based on the experimental data for evaluation of these effects. Within this work, numerical procedure for prediction of the effect of biofouling on the ship hydrodynamic characteristics is implemented within STAR-CCM+, which enable the determination of these effects.

Preliminary results
Roughness functions which can be used for the determination of the effects of biofilm on the flow around the surface covered with biofilm are proposed and implemented within commercial software package, STAR-CCM+. Afterwards, the validation study is performed in order to evaluate the effects of biofilm on turbulent channel flow. The frictional resistance coefficients obtained utilizing numerical simulations with the application of proposed roughness functions are compared to the experimental results which are available in the literature and satisfactory agreement has been achieved.

Discussion
The next step in this study includes the analysis of the effects of biofilm on the ship resistance and propulsion characteristics in calm water. The total resistance of a ship will be decomposed and thus the effects of the biofilm on each resistance component will be assessed. Furthermore, an analysis of the effects of the biofilm on open water characteristics of a marine propeller will be performed. The effect of the biofilm on ship propulsion characteristics will be assessed utilizing numerical simulations of self-propulsion test with and without application of the proposed roughness functions, and through detail analysis of resistance and open water test results.

Acknowledgments
I wish to thank professor Degiuli for her constant encouragement and support.

Keywords
Computational Fluid Dynamics (CFD), biofouling, roughness functions, resistance characteristics, propulsion characteristics
**A Fast Model for Predicting Road Transport Emissions**

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**Introduction**
According to “EU 2030 Climate & Energy Framework”, by 2030 greenhouse gas emissions resulting from road transport need to be reduced to 30% below the reference year 2005. To be able to perform these obligations efficiently and at minimum cost, the Republic of Croatia needs to have at its disposal an appropriate road transport emissions estimation model to allow an effective analysis of the possible scenarios. Unlike the common tools used to estimate emissions, which require entering large volumes of data and are therefore very time-consuming, the newly proposed model is based on the functional relation between the emissions and the relevant parameters for the entire fleet. This was used as a basis to develop a mathematical model that will allow predicting the future development of fleet emissions over the next few time steps according to the assumed scenario.

**Methods**
This research includes five phases. In Phase 1 the previous research in the field of road transport emission modeling was thoroughly analyzed. In Phase 2 the M1 vehicle fleet in Croatia was analyzed. Data about the fleet were collected as part of regular annual technical inspection and vehicle registration activities. Fleet emissions were calculated using the COPERT 5 software. Functional relation was established between the relevant fleet parameters and emissions. In Phase 3 an emission management model that will be used in the context of the intended fleet structure changes was developed.

**Preliminary results**
A regression analysis found functional relation between the relevant parameters during the observed 2007-2016 interval, whereas the situation in the reference year 2005, for which certain necessary data were unavailable, was successfully reconstructed.

**Discussion**
The new model is based on an analysis of the fleet’s emission structure, the annual mileage and the total emissions data of each pollutant, as well as on determining the functional relation between the emissions calculated by using a standard tool and the relevant parameters for the entire fleet. Phase 4 will include the application of the model to the selected scenarios and Phase 5 will be reserved for the evaluation of the extent to which the aims set were accomplished.

**Acknowledgments**
I hereby thank to the companies Inter-net and CVH regarding data analysis from the CVH database and the input data preparation.

**Keywords**
Road transport emissions, car fleet modeling, emissions management
Numerical-Experimental Suitability Analysis of Using Agricultural Biomass in Hot Water Boilers

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Introduction
Energy independency and environmental awareness have been the grounds for a rise in the use of biomass as a substitute to fossil fuels. In the industrialized world, biomass is mainly used for producing heat, either in large or medium sized district heating systems or in residential wood logs/pellets boilers stoves and fireplaces. In recent years the market for wood pellets in Croatia has stopped increasing as the cost of heating has become higher to that of natural gas. This enabled the growth of agropellets market, which are becoming more and more desirable fuel due to their lower cost compared to wooden pellets. The use of this agricultural biomass pellets is considered as viable options for the production of heat, primary due to their low cost. However, there are several challenges related to combustion of agro-fuels in small scale appliances (high particulate matter and gaseous emissions, lower combustion efficiency, ash/residue related problems).

Methods
Four pellets used in this study: wheat straw (WS), wheat straw with hazel shell (WSHS), rapeseed straw (RS) and wood (WO) are obtained from the agropellets factories situated in Croatia (Pitomača and Donji Miholjac). Information relevant to the combustion properties of obtained pellets are researched via literature survey. Laboratory measurements are performed according to EU normalization standard (EN 303-5:2012) in 20 kW high efficient/low emission wood hot water boiler (HWB) installed with 6-26 kW rotary combustion chamber burner, particularly suitable for burning of fuels with high content of non-combustible impurities. Special attention is given to the residue analysis where the mass of combustible constituents is determined and agglomeration characteristics are observed.

Preliminary results
Low ash melting temperatures of most types of agricultural residues is identified as a crucial problem in achieving an efficient combustion. Rotary combustion chamber burners proved to be particularly suitable for burning of fuels with low ash melting temperatures without the need to manually remove agglomerate or slag. Obtain results show that using WO Class 5 and using RS Class 3, according to EU standard, is achieved. WS and WSHS proved not to be as particularly suitable to burn in form of pellets the in selected installation, resulting in high amount of lumped residue particles containing large amounts of unburned carbon. This implies that existing HWBs cannot be easily modified to burn all available agropellets.

Discussion
In literature, combustion properties of agricultural biomass are mostly only explored in terms of fuel properties. Several papers analyze combustion of agricultural residues and other non-conventional biomass in various laboratory tests and/or real life performances mainly using the pellets with ash content below 3%. In contrast to the other investigations, this paper deals with combustion and emissions results obtained from tests performed according to EU normalization standard by burning of biomass pellets with very high ash content (above 5%). According to the observed results, burning applicability of various agropellets is determined and several modifications to the conventional combustion system are proposed.

Keywords
agropellets, combustion efficiency, pollutant emission
Levelized Cost of Excess Heat as a Method for the Evaluation of Excess Heat Utilization in District Heating Systems

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Introduction
District heating constantly proves to be the efficient way of supplying heat to the final consumers. Despite this fact, only 13% of the European heat supply is covered by these systems, showing great potential for further expansion. Excess heat presents a particularly interesting heat source for these systems. It represents heat from different processes, e.g. industry, service sector, which is currently being wasted. The potential for its utilization has been proved to be rather significant.

Methods
In order to utilize excess heat as a heat source in a district heating system, the feasibility of the investment should be assessed. Levelized cost of energy is often used for the purpose of comparing the investments in different energy production units. When it comes to excess heat utilization, two major investments have to be made: heat exchangers and distribution pipes. The pipes present an especially significant investment since the source of excess heat is usually located further from the demand. This has been acknowledged by implementing a two-step method. In the first step, levelized cost of excess heat is calculated. It takes into account the discounted heat exchanger investment, operation and maintenance costs and the price of excess heat. In the second step, an extra revenue is calculated by subtracting the costs of the heat production and district heating network construction from the heat sale revenues. This can be used for the construction of the distribution network to transfer excess heat to the demand. That way, maximum distance of the excess heat source from the demand can be calculated.

Preliminary results
This way, the impact of different parameters on the maximum distance from the potential heat demand can be analyzed. A sensitivity analysis has been performed by changing three different parameters: the cost of pipes, available excess heat supply and the price of excess heat. The preliminary results show that the developed method can be used as a criterion for excess heat utilization in district heating systems, taking into account both capital intensive investments: distribution pipes and heat exchangers. The cost of pipes has the highest influence on the feasibility of the system, but in all the studied cases, excess heat utilization proved to be the feasible solution.

Discussion
Excess heat proves to be a feasible heat source for district heating systems. Nevertheless, the tendency towards deregulated local heat markets should be taken into account in the analysis. Levelized cost of excess heat could be used here as well in order to model such a heat market and therefore provide the assessment of its functionality. This will be a part of the future research.

Acknowledgments
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Keywords
Levelized cost of excess heat, district heating, excess heat, environmental impact, energy planning
Influence of Chemical Composition on Al-2.5Mg-0.7Li Alloy Microstructural Constituents Development

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**Introduction**  
Since the application of aluminum (Al) alloys was expanded to lightweight materials with demands for high strength and stiffness to weight ratio, lithium (Li) and magnesium (Mg) were recognised as a principle (major influencing) alloying elements. Interaction of Li and Mg additions influences on microstructural constituents’ development during solidification. Consequently, the mechanical properties of Al-Mg-Li alloys are revealed as a result of developed microstructural constituents due to element interaction, present thermodynamic parameters and therefore solidification sequence.

**Methods**  
The Al-2.5Mg-0.7Li alloy was synthesized in an induction melting furnace under protective atmosphere of argon (Ar) and crucible cover. Solidification sequence under equilibrium conditions was identified using Computer aided thermodynamic diagram calculation (CALPHAD). The influence of different heating and cooling rates on phase transformations and precipitations was determined using Differential Scanning Calorimetry (DSC). Microstructural constituents were identified using different techniques of metallographic analysis. Correlating the results of CALPHAD, DSC and metallographic analysis enabled determination of microstructural constituents’ development in non-equilibrium conditions.

**Preliminary results**  
Solidification sequence of Al-2.5Mg-0.7Li alloy under equilibrium conditions, involves transformation of liquid into primary dendrite network $\alpha_{Al}$ phase followed by precipitations of ternary $\text{Al}_2\text{LiMg}$ (T) phase and $\text{Al}_5\text{Mg}_5$ ($\beta$) phase.

Solidification sequence under non-equilibrium conditions begins with transformation of $\alpha_{Al}$ phase. Development of $\alpha_{Al}$ dendritic network is followed by eutectic precipitation of metastable $\text{Al}_3\text{Li}$ ($\delta'$). Stabile $\text{AlLi}$ ($\delta$) phase nucleates on the grain boundaries of $\alpha_{Al}$. Reaction between bulk $\alpha_{Al}$ and $\delta'$ phase enables precipitation of ternary T phase on the grain boundaries as well as inside the grains. Solidification sequence ends with precipitation of secondary eutectic $\beta$ phase on the grain boundaries.

**Discussion**  
The significant difference between solidification sequences in equilibrium and non-equilibrium conditions is a result of chemical composition and thermodynamic parameters influence. Mg reduces solubility of Li in Liquid phase (L) and $\alpha_{Al}$. Reduced solubility of Li in L phase leads to eutectic precipitation of $\delta'$ phase inside the $\alpha_{Al}$ grains. Cooling, constitutional undercooling and therefore reduced solubility of Li in $\alpha_{Al}$ causes precipitation of $\delta$ phase. Precipitation of T phase is a result of reaction between $\alpha_{Al}$ enriched in Mg and $\delta'$ phase. Solidification sequence ends with precipitation of $\beta$ phase followed by decrease of Mg content of $\alpha_{Al}$.

**Acknowledgments**  
This investigation has been performed in the frame of Financial support for investigation of University of Zagreb: „Design and characterization of innovative engineering alloys“(TP167) and support of scientific research projects within the joint Croatian

**Keywords**  
Al-Mg-Li alloy, magnesium, lithium, solidification sequence, non-equilibrium conditions, microstructural constituents
The Novel Model for Monitoring the Human Factor Efficiency in Processes

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Introduction
Modernization and digitalization, which are society demands, affect on many processes. Accordingly, modern technologies are changing the entire way of doing business both in professional and in academic organizations. A prerequisite for introducing new technologies is the waste elimination within the process. The fact is that any involvement of a human factor within the process, besides subjectivity, also causes a human error which may be intentional or unintentional. In order to identify anomalies and to prevent any manipulation within the process, the new technologies application proposes an excellent solution. For this purpose, the aim of this research is to develop a novel model that will provide human factor efficiency monitoring and improving within various processes on the case study example of monitoring employees in periodical technical inspection stations and making decisions regarding their performance.

Methods
In order to investigate research area, the literature review was made first. Also, the process was analyzed regarding lean concept methods. Furthermore, the data from database was collected and relevant parameters were determined according to data analysis. To determine the relation between the parameters and their impact on the response, the binary logistic regression was conducted because the response variable was dichotomous.

Preliminary results
According to a literature review, although the lean concept and industry 4.0 are closely related to production industry, there is an increasing tendency of their implementation in other types of industries. However, it is necessary to adjust the existing lean conceptual model for application within the process where the emphasis is on the human factor. Determination of relevant parameters was obtained by defining rules for decision-making by use of statistical analysis. Regarding decision-making, expert system implementation, which was presented in one conference paper, is of great importance for decision-making support. However, it is quite clear that subjectivity is difficult to measure because decisions are often made based on instinct and experience. For this reason, the emphasis is on determining parameter values that can indirectly indicate errors and defects within the process.

In order to achieve more accurate model, more effort has to be made in data analysis and more parameters should be further investigated.

Discussion
The next step will include more detailed data analysis by the method that will be determined during the research. Also, the analysis of the process will represent the base for the digitalization of the decision-making process regarding human factor evaluation. The purpose of this research is to intersect the lean concept analysis of the process, the data analysis and new technology implementation to achieve a more efficient process of the efficiency evaluation.

Acknowledgments
I would like to thank to CVH (The Center for Vehicles of Croatia) company for supporting and providing this research.

Keywords
data analysis, human factor, lean concept, industry 4.0
Development of a Numerical Model for the Evaluation of the Ship Added Resistance in Waves

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**Introduction**  
Evaluation of the ship added resistance in waves has increased in importance, especially from the economic as well as from the environmental point of view. Ship added resistance in waves causes a reduction in ship speed and has an impact on the increase in the fuel consumption as well as on the emission of harmful gases, which is subject to the increasingly stringent regulations. The determination of the ship seakeeping characteristics and added resistance in waves requires rather complex hydrodynamic calculations. Therefore, it would be beneficial to develop a model that would allow for a simple but sufficiently accurate and reliable evaluation of the added resistance in waves at an actual sea state. This is especially important in the ship design phase or while planning a favourable sailing route of a ship in service. One of the possible tools for the establishment of such a model are artificial neural networks, which have the ability to learn from examples and to identify relationships between the input data and solutions to the multivariable problems.

**Methods**  
Within this research, a large number of hull forms will be generated and the influence of mass characteristics and hull form parameters on ship added resistance in waves will be investigated. Feedforward neural network with static neurons and error-back propagation algorithm will be generated, and input parameters will be evaluated and proposed. Panel method will be used for the determination of added resistance in waves to define the optimum architecture and learning parameters of the neural network, as well as for training of the network in the first stage of the research. Ship added resistance in waves for actual sea states will be determined based on the numerical results for regular waves and by means of irregular waves energy spectrum. The numerical results obtained by hydrodynamic calculations and the output of the proposed neural network will be validated against the available experimental data.

**Preliminary results**  
A database of hull forms that represent typical forms of modern containerships is established. A number of the hull forms, required for hydrodynamic calculations, is generated and prepared as an input for both potential and viscous flow solvers. Verification and validation of the potential flow solver are performed for the benchmark ships. In addition, the influence of ship mass characteristics on added resistance in waves is investigated. Basic form of feedforward neural network with error-back propagation algorithm is generated as well.

**Discussion**  
Validation of the potential flow solver showed satisfactory accuracy of the results regarding ship added resistance in waves for slender hull forms in the range of moderate and long relative wavelengths. The optimum architecture of neural network as well as learning parameters will be set based on the numerical results obtained using potential flow solver, i.e. panel method. The influence of the hull form parameters on ship added resistance in waves will be investigated and input parameters for neural network will be evaluated and proposed. Verification and validation of viscous flow solver will be performed for the benchmark ships. An optimum simulation setup as well as grid density will be defined regarding the numerical accuracy and minimization of the computational time and resources.

**Acknowledgments**  
I wish to thank professor Degiuli for her constant encouragement and support.

**Keywords**  
Added resistance in waves, Computational Fluid Dynamics (CFD), neural network, seakeeping characteristics
Enhanced Model for Organizations’ Carbon Footprint Calculation

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**Introduction**  
The establishment of a harmonized approach for calculation and reduction of carbon footprint (CF) on global level is an important part of possible solution for climate change mitigation. The CF represents the total amount of greenhouse gas (GHG), directly and indirectly, emitted in the atmosphere by a project, a person, an event, an organization, or a product.

**Methods**  
In the framework of research, an enhanced model for CF calculation of organizations was developed, based on the IPCC methodology, Life Cycle Assessment approach and French Bilan Carbon® tool. The existing model is extended with the national emission factor database. The model will be improved by incorporating the criteria for CF comparison and new module for analysis of GHG emission reduction measures. The model completely follows the appropriate international standards (GHG Protocol and ISO standards) and will be applicable in different climatic and socio-economic regions.

**Preliminary results**  
The model was already tested on the case of Energy Institute Hrvoje Požar. The Institute’s CF were calculated for 2015 and 2016. The CF calculation takes into consideration all flows of energy, materials and people, necessary for the functioning of the Institute. Footprint was larger in the last analyzed year, due to increased number of employees. Scope 1 activities (direct emissions and emissions from Institutes’ cars) contribute only 5-6% to the EIHP’s CF. Scope 2 activities (the electricity and heat consumption, produced outside the Institute) cover about 23-24%, while more than 70% of the total GHG emissions belong to Scope 3 activities. The most important source category was transport of people. Commuting of employees, business travels and visitors’ travels cover more than 50% of EIHP’s carbon footprint.

**Discussion**  
The calculation of the CF is an important first step, which will allow organizations to become more familiar with their emission structure and recognize activities that mostly contribute to the total GHG emissions. Using this enhanced model, a CF will be calculated for 5-8 organizations from the public and private sectors. In addition to the CF calculations, action plans for CF reduction will be prepared for at least three selected organizations. In the plan, the short and long-term goals will be defined, as well as the cost-effective measures for achieving defined goals. Finally, the whole process should be finished with implementation of GHG emission reduction measures, recognized in the action plan.

**Acknowledgments**  
This research is the part of the Clim’Foot project „Climate Governance: Implementing public policies to calculate and reduce organizations carbon footprint“, co-financed through the LIFE program. This help is gratefully appreciated.

**Keywords**  
carbon footprint, greenhouse gas emissions, IPCC methodology, Life Cycle Assessment, Bilan Carbone® tool
Two-Scale Damage Model for Quasi-Brittle Heterogeneous Materials

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Introduction
In recent years it has been shown that the conventional homogenization approach is not appropriate for the objective multiscale analysis of the softening materials, because the averaging over the whole representative volume element (RVE) cannot adequately describe the localization phenomena. Besides, instead of the converged homogenized solutions, increase in the RVE size leads to increasingly brittle structural responses observed on the macroscale. There are some suggestions to overcome these problems, where the converged results are obtained by averaging only over a propagating damaged zone in the RVE. Derivation of an efficient and accurate multiscale method is still under development.

Methods
In this contribution, an existing two-scale model employing the nonlocal strain gradient theory at both micro- and macrolevel is extended and transformed to the analysis of the softening materials. The discretization of both levels is performed by means of the C\(^1\) continuity triangular finite elements. The damage model, based on the strain gradient continuum with an exponential evolution law describing the softening of quasi-brittle materials, is implemented at the RVE level. Two separate analyses are performed there, one for the undamaged bulk, where the stress and constitutive operators are extracted using the conventional homogenization, and the other one for the softening material, where the localization is captured by a novel approach. Herein, the damage variable is homogenized only over a loading zone where softening is progressing. Since a linear-elastic material is used, the bulk constitutive operators remain unchanged throughout the analysis and therefore can be computed only once. The degradation of the macroscale stiffness is governed by the isotropic damage law employing the homogenized damage variable.

Preliminary results
The verification of the presented damage model is made on a benchmark example consisting of a rectangular plate with an imperfect zone under tension. The results obtained are compared with the solutions acquired using the one-scale model, where the identical damage model as used at the RVE level in the two-scale analysis is employed. In the case of homogeneous material, both approaches yield similar damage distributions over the plate, while differ significantly in structural response, i.e. when the force-displacement curves are compared. Analyses considering heterogeneous materials are still under investigation.

Discussion
Strain localization and softening phenomena can successfully and efficiently be captured by means of the proposed multiscale computational strategy. Although the same damage evolution law is used at the microlevel in the two-scale analysis as in the approach where only one-scale is considered, it is obvious that the novel homogenization technique affects the macroscale structural behavior by making it more brittle.

Acknowledgments
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Keywords
Quasi-brittle damage, Homogenization, Multiscale analysis
A Phase-Field Staggered Algorithm for Brittle Fracture Modelling

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Introduction
In the classical continuum mechanics, numerical damage and fracture modelling leads to the mesh density and mesh orientation dependent results in the framework of finite element method. The reason is the inevitable loss of ellipticity of the system’s governing equations on the onset of the deformation localization and material softening. In order to circumvent the non-physical behavior of standard models, various approaches have been proposed incorporating an internal length measure as a common feature. A very promising which gained a lot of publicity lately is the phase-field fracture modelling method. It is based on a variational principle of the energy minimization as an extension of the Griffith’s brittle fracture theory. Instead of the numerical tracking of the sharp-crack surfaces used by the discrete crack modelling methods, it introduces a scalar damage field, called the phase-field, which distinguishes between the cracked and intact material states. That way, the numerical implementation complexity is vastly reduced. Moreover, what makes this approach particularly attractive is its thermodynamic consistency and its ability to simulate arbitrary complex fracture phenomena even on three-dimensional problems.

Methods
Due to the non-convexity of the phase-field free energy functional, a robust staggered solution scheme based on the operator split is typically used. This research deals with the implementation of the staggered phase-field algorithm for brittle fracture modelling into the commercial finite element software ABAQUS by the means of the UEL and UMAT subroutines. The phase-field parameter is introduced in the formulation as an additional degree of freedom whose evolution is driven by the elastic deformation energy.

Preliminary results
The presented implementation is verified on the several standard benchmark examples, including the homogeneous plate for which the analytical solutions are known as well as the mode I and II fracture problems. The obtained results are compared with the experimental and numerical results from the literature in terms of accuracy, robustness and computational costs.

Discussion
The obtained results match well with the experimental data and the numerical solutions from literature. Moreover, compared to the existing ABAQUS implementations of the phase-field fracture modelling, the presented implementation demonstrates an improvement in the computational efficiency. It is developed as a framework for the future extension of the formulation to the ductile fracture settings as well as the heterogeneous materials modeling through the multiscale numerical procedures.

Acknowledgments
This work has been fully supported by Croatian Science Foundation under the project Multiscale Numerical Modeling of Material Deformation Responses from Macro- to Nanolevel (2516).

Keywords
phase-field modeling, fracture, staggered algorithm, ABAQUS
Industry 4.0 Readiness Factor Calculation Overview

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Introduction
Digitalization era is not in front of us, but it is a present state which industry must embrace as new everyday working environment. In European countries the result of the digitalization process is well known as „Industry 4.0“.

Changes of some kind must happen for company to stay competitive on the market. Changes happen both in the hardware, software, but also in the psychological approach of the human workers which must adapt to new situation and get the most out of it for the well-being of the company. Their education is very important, because the transformation happens also in the traditional professions which will change with the input of the new ones, that haven’t been present so far. The problem with the transformation is the resistance to change and the fact that the very same change demands financial investments of some kind. That is why before the actual transformation the readiness factor of the company should be calculated to get an overview where the certain company is now, compared to what should be achieved. The literature review of the readiness factor calculation methods will be presented, and the idea for readiness factor calculation by multicriteria decision support will be presented with its advantages and disadvantages.

Methods
The readiness factor helps to create investment/transformation plan/project more effectively and with less cost of the future actions. Because the change has big impact on the company’s future, the appropriate readiness factor calculation method should be used, but also in a short time with minimum cost. The decision support systems allow an approach based on multiple criteria and the problem structuring by the unique needs of the user. One of the multicriteria decision support methods that will be used for readiness factor calculation is Analytic Hierarchy Process (AHP method).

Preliminary results
In the first stage of the research the conclusion was made that there are several methods for readiness factor calculation already existing, but they are all based on the level of the industrial revolution company is in. With the new approach the more detailed overview and grade could be given, judged in every department of the company separately.

Discussion
After the method testing the basic criteria tree must be completed that can also be customized easily for the needs of the certain user. Apart from the AHP method, the other multi criteria decision support systems have to be tested.

Keywords
Industry 4.0, readiness factor, DSS, AHP
Two-Way Coupled Euler-Euler Simulations of Particle-Laden Flows

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Affiliation: Binkz Inc, Canada

Introduction  
A novel two-way coupled Eulerian-Eulerian CFD formulation for simulating particle-laden flows using the Finite Volume Method is presented.

Methods  
The presented approach is based on a new viscous model of the particle phase, and turbulent dispersion through a turbulent drag term in the phase-averaged momentum equations. This approach allows explicit resolution of both saltation and suspension layers without resorting to empiricism, unlike other one-way coupled Eulerian-Eulerian approaches based on mixture formulations using the convection-diffusion particle transport equation, or the Volume of Fluid method.

Preliminary results  
Successful validations are carried out against detailed measurements from controlled experiments of drifting snow. The present two-way coupled approach is found capable of accurately predicting snowflux and airflow profiles. Comparison is also made to the results of a one-way coupled method based on the convection-diffusion equation for transport of solid sediment. Both approaches are used for simulating an experiment of sediment suspension in a laboratory flume. The two-way coupled approach is shown capable of accurately predicting both sediment concentration and water velocity profiles, more accurately than the one-way coupled approach. The present two-way coupled approach is also shown capable of accurately predicting the sediment fall velocity and wall effect, without the need for the empirical relationships used for the one-way coupled approach that predict a constant sediment fall velocity throughout the entire computational domain.

Discussion  
The present two-way coupled approach is found more accurate than existing one-way coupled approaches, while not relying on empirical formulations. It is desirable to extend the present approach to handle several particle diameters simultaneously. It is also desirable to investigate the effect of particle collisions within particle beds, as well as particle bonding, both effects being presently implicitly included in the surface threshold shear stress term. Validations against flows around buff bodies are also desirable since such flows routinely occur in real life situations.

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Keywords  
euler-euler, multiphase, particle-laden flow, two-way coupling, one-way coupling.
Relaxation Behaviour of Poly(Vinyl-Alcohol)/chitosan Blend with Different Compositions

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Introduction
Polymer blends are materials in which at least two or more structurally different polymers are blended together in order to create a new material with properties that cannot be achieved in a single polymer. The properties of blends depend on the properties of their constituents, their morphology and interfacial characteristics. A combination of natural and synthetic polymers can be an effective way to produce blends with many desired properties. This research focuses on relating structure and thermo-mechanical properties of polymer blends with different compositions. Organic nanoparticles of chitosan (CS) with antimicrobial activity are added in a non-toxic poly(vinyl-alcohol) (PVA) matrix. Chitosan is second most abundant natural polysaccharide next to cellulose and is well known for its biocompatibility and biodegradable properties. It is non-toxic, so that, it is preferred to be used in biomedical applications. Since it contains hydroxyl and amine groups, it is miscible with flexible PVA due to the formation of hydrogen bonds. PVA is water soluble, non-toxic, biodegradable and biocompatible synthetic polymer with good mechanical and excellent film forming properties which is widely used in biomedical field. CS reduces the crystallinity of PVA in the mixture which causes degradation of mechanical properties. However, the properties of the polymer matrix can be improved by chemical crosslinking with glutaraldehyde (GA) which reduces the negative effect of CS on PVA properties.

Methods
Various blending ratio of PVA/CS blend films were prepared by solution blend method. A 5 wt% PVA aqueous solution was prepared by mixing fully hydrolised PVA and distilled water. A 1% acetic acid solution was used to prepare a 2.5 wt% solution of low molecular CS. The blend is chemically cross-linked by means of the glutaraldehyde. The resultant PVA/CS solutions are casted in glass moulds and then dried in oven in order to prepare thin flexible films. The thermo-mechanical properties of the PVA/CS blend films were examined by means of dynamic mechanical analysis (DMA).

Preliminary results
Results of the analysis are shown in mechanical spectra. Loss factor \( \tan \delta = E''/E' \) shows the \( \alpha \) relaxation peak that is associated to the glass to rubber transition of the amorphous phase, and is controlled by both intra- and intermolecular interactions. When CS is added to the PVA, the intensity of the relaxation increases. CS reduces the crystallinity degree leading to the higher amount of the amorphous phase that contributes to the \( \alpha \) relaxation process. However, a slight drop and shift to higher temperatures is observed when PVA/CS mixture is chemically crosslinked because crosslinking restricts mobility of the amorphous phase. The relaxation peaks in the mechanical spectra are broad that indicates an increase in heterogeneity in the structure.

Discussion
DMA analysis of polymer blends is of great interest and importance, resulting from its great sensitivity in detecting changes of internal molecular mobility. From different relaxation processes visible on \( \tan \delta \) curve in DMA spectra information about structure and mechanical properties depending on temperature can be obtained. In addition to the DMA, future work will include other methods for thermal and structural characterization such as DSC and FTIR analysis.

Keywords
Polymer blends, glass transition, dynamic mechanical analysis
Influence of Design Requirements on the Spur Gear Pair Parameter Selection

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Introduction
Modern day products are expected to perform their function without error. For this reason, additional desirable features are required to gain a competitive edge. Examples of such features for geared transmissions are lower weight, compact dimensions, high efficiency and low noise levels. The often opposing additional criteria in addition to the elaborate calculation procedure yield a difficult design task, requiring expert knowledge. A resulting task is often solved using either the theoretical, numerical or experimental methods. The research aim is to develop a procedure for spur gear pair optimization applicable when multiple additional objectives exist. This procedure will be suitable for both steel and polymer gears, enabling a comparison between the two. The influence of the gear module, face width, profile shift factors and teeth number on the gear pair volume and power losses will be assessed.

Methods
The first research phase is theoretical and aimed at the steel gears. To determine the number of required variables, gear strength calculation method will be integrated into an optimization algorithm. After determining the number of variables, a multi-objective procedure will be developed, with objectives being lower weight and lower power losses. Expressions for power loss calculation will be modified to enable integration into the existing algorithm. For polymer gears, a procedure will be developed using the same variables. Experimental measurements of friction coefficient will be carried out to enable the power loss calculation. The influences of load, curvature radii and sliding velocity will be analysed.

Experimental verification will be carried out in the second phase. Resulting Pareto optimal gear pairs will be manufactured and examined using the open-circuit device. Measured power losses will be compared against the theoretical.

Preliminary results
Preliminary results have shown that use of five variables is required. In addition to the gear module, face width and pinion teeth number, profile shift coefficients ought to be used. Single-objective optimization has shown that including the profile shift factors as variables enables the volume reduction up to 34%. Modified power loss formulae were implemented into the multi-objective optimization algorithm (NSGA-II was used). Results have shown that the increases in the gear module, the wheel profile shift and the face width will decrease the power losses. Solutions with the lowest volume tended to have the high pinion profile shift. Lastly, all the solutions converged towards the larger pinion teeth number.

Discussion
Results for the steel gears are in the agreement with the existing literature. Even though the designer has to choose the final solution from the set of Pareto optimal ones, use of the proposed procedure significantly decreased the time spent. It should be noted that the dynamic transmission error (DTE) was not considered since the suitable analytical expression was not found.

Keywords
Gear, multi-objective optimization, power loss, genetic algorithm, polymer gear
Design for Additive Manufacturing with Mapping of Product Functions

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Introduction
Design for Additive Manufacturing (DfAM) is a new engineering practice that utilises unique manufacturing capabilities of additive manufacturing (AM) to achieve desired performance and new functionalities of a product. Hitherto developed DfAM methods are focused on utilising AM possibilities through redesigning of existing products in detail design phase with little or no consideration for early phases of product development. To develop genuine AM products, it is necessary to implement AM knowledge in early phases of product development process. Here one of the essential tools is functional decomposition where the overall function of a product is decomposed in all its subfunctions. For such subfunctions, it is easier to find a partial solution for a given problem. Therefore, this research proposes a new method for mapping product functions with design principles for AM, to help designers find different solutions for a function or block of functions when developing an AM product.

Methods
The research methodology consists of four phases: preliminary research, data gathering, data model realisation and evaluation. In preliminary research overview of existing scientific and expert literature was conducted. The focus of literature overview was on early design phases and influences of AM, as well as on fabrication capabilities of AM processes. Literature overview defined basic presumption, research goals, main research question and hypothesis. The second phase will be focused on data gathering where existing products and artefacts produced with AM will be evaluated to extract and establish the initial database of AM principles. In the third phase, a theoretical data model for mapping of functions and design principles will be developed, as well as a computer framework with tools for performing the mapping. The final phase will include evaluation through case studies for validation of AM design principles database and user studies for validation of the proposed methods and tools.

Preliminary results
For initial verification of basic presumptions, a case study was conducted where we used the proposed method to develop a continuous flow microreactor. In conceptual phase of microreactor development, functional decomposition of microreactor was mapped with design principles for AM. This enabled the creation of a concept that, based on the given design principles, utilise different AM possibilities and integrates them to achieve desired performance and functionality. The final design was transparent one-piece microreactor with a complex internal geometry. Testing showed that product successfully fulfils all functions that are necessary for successful mixing of fluids and monitoring of the reaction process.

Discussion
Preliminary results showed that the method enables mapping of product functions with design principles for AM, it offers partial solutions for the given problem and enables function integration. The method utilises the AM knowledge in early design phases and enables development of AM products. Therefore, the future research will be focused on the development of AM design principles database and computer framework for performing mapping of product functions with design principles for AM, as well as its validation.

Keywords
additive manufacturing, functional decomposition, design principle, product development
Introduction
By development of modern methods such as thermography and the visioplasticity with digital image correlation simultaneously using the static tensile test problems that occur with inhomogeneous deformations, i.e. Lüders bands, during cold deformation are topical in recent times. For the purpose of Lüders bands clarification, the influence of certain influential parameters on Lüders bands formation and propagation on various metal materials was investigated. There are differences in the chemical composition and initial microstructure as well as differences in test conditions such as different strain rates. Therefore, it is not possible to clarify the differences in the interpretation of certain influential parameters on the Lüders bands formation and propagation.

Methods
Research on microalloyed steel with different niobium content will be conducted. Special attention in research will be on the Lüders bands formation and propagation at the beginning of plastic flow of material. Stresses, as well as Lüders strains, in the deformation zone during Lüders bands formation and propagation will be determined by using modern methods thermography and digital image correlation during the static tensile test. Influence of microstructure at the beginning of plastic flow of material will be research with structural studies. The impact of the different niobium content, and the size and distribution of niobium precipitates at the beginning of plastic flow of material will be determined with optical microscope, scanning electron microscope, and transmission electron microscope.

Preliminary results
On microalloyed steels with different niobium content (0.035 wt. % to 0.06 wt. %), preliminary tests using static tensile test, thermography, digital image correlation and structural testing with optical and scanning electron microscopes were performed at different strain rates. Preliminary results of performed tests show the influence of the initial structure of the steel in such way that in samples with nonhomogeneous structure and the higher content of the pearlite Lüders bands did not appear, while in the samples with the homogeneous structure and the lower content of the pearlite Lüders bands appeared.

Discussion
Different niobium content has an influence on the Lüders bands appearance and propagation. The next steps of the research are to determine the mechanism of Lüders bands formation and propagation in niobium microalloyed steel with modern methods digital image correlation and thermography. Experimental results from structural studies should clarify the role of size and composition of niobium precipitates on the Lüders bands appearance and propagation.

Acknowledgments
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Keywords
Microstructure, Lüders bands, static tensile test
Design of Smart Product

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Introduction
Industry 4.0 changes the practice in manufacturing. Integrating production machines with information technology outlines a trend of “smart product” development. Better controllability, adjustability and integrability with another technical system in modern industrial environments offer added value to this kind of products. Basic characteristics of smart product arise from smart components which embed knowledge of its function, behavior and structure. Smart sheet metal forming tools are one specific segment of smart products. Controllable actuators in direction different from the press opening and sensors that give information about work pieces, tools and process regulate the production process parameters in real time. The production is more competitive because it delivers at lower costs with increased safety and meets customer needs with more flexibility. Smart product design process models should enable the integral processing of complex requirements that exist in such a process. They should include information processes throughout the product lifecycle as a source of product information in real time.

Methods
An understanding dynamic process of product development and design is a very demanding task. There are two important aspects of the presented research: (1) differentiation between theoretical framework of the existing methods and empirical models context of design process depending of context of developed product) and (2) examination of real smart product design process, not only or theoretical correctness, but also applicability of the method in the context of application.

Preliminary results
Results of the preliminary literature review indicate that there are enormous needs for research in the field of smart technical systems development and design. A methodological approach to the development of any kind of product in industry is partially practiced. The real successes of applying the methodology in industrial product development can only be found in a limited number of published examples which are often the result of cooperation between universities and industrial partners. The same is in smart sheet metal forming tools field. This results will be compared with the situation in respected sheet metal tools making company.

Discussion
The research aims to develop a model to support the design process that will enable integrated processing of complex design requirements, including the information processes throughout the product lifecycle. The evaluation of research outcomes will incorporate: the analysis of the data collected in the real process of developing smart sheet metal forming tools using a proposed model, analysis of advantages and disadvantages of the proposed model and comparison of the achieved results against the defined research goals.

Keywords
Smart product design, smart sheet metal tools, design theory, product development
Data Preparation and Description Prior to Machine Learning Analysis

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**Introduction**  
Following the regulation of EU Directive on Energy Efficiency, specifically Article 9, individual metering in district heating systems has to be implemented in all EU Member States by the end of 2016. The Directive allows installation of both heat metering devices and heat cost allocators. Mainly due to bad communication and PR in Croatia, the general public false image was created that the heat cost allocators are devices that save energy. Although this notion is wrong, the aim of this work is to develop a model that would precisely express the influence of installation heat cost allocators on potential energy savings in each unit within multifamily buildings.

Previous work has shown that the expected savings can be expected on the level of approximately 25%. The intention of this paper is to identify a machine learning algorithm that best estimates the actual savings.

**Methods**  
The direct hypothesis is that the collected data is representative and that their interrelationship, meaning the correlation, data group, distribution, etc., will provide a good estimate on the actual benefits of installing individual metering in district heating systems.

Experimental research is conducted on a set of actual energy consumption data for the City of Osijek.

The pre-processing of the available data was made, together with the statistical analysis. Furthermore, the data sampling was conducted. In this paper the data processing prior to undergoing the algorithms’ comparison is given.

**Preliminary results**  
Preliminary results show that the data composition is normal, and in line with the expected results based on the experience with processing data in other district heating systems (other EU countries, besides Croatia).

**Discussion**  
Data analysis should be implemented on the data for another town with district heating, expecting to get the same results. This is to be done in the next step.

**Keywords**  
data preparation, statistics, district heating, energy efficiency
Advanced Planning of Energy Self-Sufficient Wider Urban Areas Using Smart Energy System Approach

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Introduction
The Republic of Croatia encourages penetration of renewable energy sources (RES) into the power system, in order to reduce pollution, encourage the exploitation of its own natural resources and to achieve the independence of the energy sector. In accordance with the above, this research will be carried out in the field of energy planning for the selected Dubrovnik region. The plan is to provide energy plan models by the year 2050 which will be based on the 10 minute data input, using advanced planning and smart energy system approach. The aim is to prove that the energy system, with 100% share of RES in energy production, could be self-sufficient, including the replacement of all conventional vehicles with electric vehicles (EV), as well as providing additional storage facilities by transforming power to heat and to cold and replacement of two-tariff model in electricity prices with the electricity market.

Methods
Borders of the selected energy system of a wider urban area are defined with the general definition that can be applied to other regions. Defined borders determine input data for the energy plan model of the selected region. Calculations are done in EnergyPLAN model, which is a deterministic input/output model for Energy Systems Analysis and runs on an hourly basis, and compared with the new algorithm based on the 10 minute time step data with regulation of energy flows according to the electricity prices on the wholesale market. Comparison of the two models will show that the 10 minute model provides better opportunities for the integration of RES in energy system using fast charging and additional electricity storages through power to heat and to cold.

Preliminary results
Energy Plan model done for the Dubrovnik region for the year 2050, based on the 1 hour time step using existing two tariff model on electricity prices, considering 100% production form RES and replacement of all conventional vehicles with EVs, resulted in a high amount of critical excess in electricity production (CEEP) and maximum peak demand. Even a slight change in variability of existing tariff model resulted in decrease in CEEP and maximum peak demand. Future work will analyse energy plan model till 2050 for the selected region which will be based on the 10 minute time step data with regulation of energy flows according to the electricity prices on the wholesale market. Comparison of the two models will show that the 10 minute model provides better opportunities for the integration of RES in energy system using fast charging and additional electricity storages through power to heat and to cold.

Discussion
Development of a new model will result in reducing the need for the additional flexibility in the system and providing more opportunities for stable integration of 100% share of RES in the energy system. Integrated electricity market model, based on the 10 minute time step of trade, will ensure the stability of the system and regulation of energy flows, enabling market valuation of flexibility sources in the system. Cost-effective participation in the system for all its participants can be achieved using information and communication technologies.

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Keywords
Energy Planning, Electric Vehicles, Renewable Energy Sources
Modeling of Material Responses Using Atomistic Submodel

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Introduction
Due to the limitations of the classical continuum mechanics finite elements method (FEM) stress calculation fail at the geometrical features with sharp edges. By refining finite element (FE) mesh in those areas there are convergence difficulties in getting the accurate stress values. However, such sudden changes in the geometry are usually present on just a couple of places within the model space so corrections of the FE’s does not have to be done on the whole model box, but only locally in the area of special interest. Since the properties of the material rest on the atomistic structure, it seems natural to bypass the problem of singularity contained within FEM by modeling those parts of system atomistically using molecular mechanics. In proposed approach idea is to place atomistic submodel (AS) in critical areas to acquire accurate stress values.

Methods
Coupling between the atomistic and continuum model is done by transferring displacement from the FE model onto AS by capturing displacement field on the edges of AS. After determining displacement atoms along the edge of AS are fixed and act as boundary conditions. The atomistic system is then analyzed at the temperature of absolute zero by molecular statics (MS) using conjugate gradient method. In MS analysis of the atomistic structure boils down to finding the minimum of potential energy landscape by increment iterative procedure.

Basic model on which procedure is tested is a simple atomic chain (AC) subjected to stretching modeled by writing own code in the software surroundings of MATLAB. Atomic interactions are described with Lennard-Jones (LJ) potential fitted to describe behavior between atoms of argon at temperatures closed to absolute zero.

Preliminary results
In the analysis of simple AC agreement between the complete atomistic model and AS has been achieved. However special attention needs to be dedicated to picking a good range of interaction when implementing interatomic potential into the MATLAB code since the sum of small values of long-range interactions can cause the pronounced nonlinear behavior of the AC which cannot be captured by simple truss FE.

Discussion
The aim of the research is to develop a simple academic model of crystal which is suitable for assessment of important parameters of atomistic to continuum coupling. By using the simple LJ potential focus can be placed on improving coupling procedure. Our ultimate goal is to utilize the best from both worlds, speed of FEM calculations and catching of relevant atomistic material features by using molecular dynamics, where continuum approximation fails.

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Keywords
Atomistic modeling, Molecular mechanics, Atomistic submodel, Atomistic to continuum coupling
Finite Area Algorithm for Thin Film Cavitation in Open Foam

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Introduction
Numerical algorithm for calculating thin film cavitational effects is presented in this study. Thin film cavitation is a common phenomenon in diverging parts of thin film contacts, such as: journal bearings, seals, lubricated metal forming, etc. Locating and calculating cavitational effects during the operation of machinery is important for their applicability, efficiency and safety. The implemented algorithm is capable of capturing both rupture and reformation boundaries during cavitation, thus being mass conserving. The implemented algorithm is validated on several test cases: single parabolic slider (1D), twin parabolic slider (1D), microtexture pocket bearing (2D) and dimple seal bearing (2D).

Methods
In the current method thin film flow is calculated using Reynolds equation. Reynolds equation is a 2D partial differential pressure equation used for calculating thin film flows between two surfaces in relative motion, with the following assumptions: fluid viscous forces dominate over body, inertia and surface tensions forces; fluid film curvature can be neglected; variation of pressure across the fluid film is negligibly small. In the current implementation Reynolds equation is discretised using Finite Area Method embedded in OpenFOAM framework. Finite Area Method is a two-dimensional equivalent of Finite Volume Method which takes into account surface curvatures. Discretisation is performed on user selected patches of computational mesh, with values calculated at face centres and fluxes at edge centres of each finite area face. The implemented cavitation algorithm iteratively identifies cavitating and non-cavitating regions of computational domain according to the pressure values calculated by Reynolds equation. Boundary faces between two zones are identified as either rupture or formation boundaries based on film flux directions at edge centres.

Depending on the type of cavitation boundary, computational matrix is modified accordingly, in order to represent rupture and formation cavitational effects. The implemented model enables calculation of pressure without numerical underrelaxation, thus being significantly faster compared to the existing finite difference model used for validation.

Preliminary results
The results of the implemented thin film cavitation model are compared to the existing 1D finite difference model for two cases: single parabolic slider and twin parabolic slider. The results show excellent agreement between the two models, and the difference is decreasing with increasing mesh density. The results of the two-dimensional microtexture pocket bearing again show very good agreement with the available literature, as well as the two-dimensional dimple seal bearing case.

Discussion
The implemented thin film cavitation algorithm shows very good agreement with the existing finite difference model, and with the available literature. Also, calculation time of the algorithm is order of magnitude smaller compared to the finite difference model. The implemented model enables fast and accurate calculation of the thin film flow with cavitational effects.

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Keywords
Cavitation, Reynolds Equation, Finite Area Method, OpenFOAM