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TEchMA2020

3rd International Conference on Technologies for the Wellbeing and Sustainable Manufacturing Solutions

Aveiro, 23rd of January 2020

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Aveiro January 23th 2020
The Director,
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TEchMA2020

3rd International Conference on Technologies for the Wellbeing and Sustainable Manufacturing Solutions

Book of abstracts

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SUSTAINABLE MANUFACTURING SOLUTIONS

A low-cost device to determine the hole expansion ratio and the Erichsen cupping index

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Abstract— The hole expansion test (HET) and the Erichsen cupping test (ECT) can be used for routine evaluation of sheet metal mechanical behavior. These formability tests require fewer quantities of material and easy specimen preparation with a fast analysis of results. The HET and ECT procedures provide a proper evaluation of sheet material stretch-flangeability, strength, and ductility. The HET consists of expanding a hole employing a punch with a conical-tip through a die, aiming to form a flange around the periphery of the hole [1]. The stretch-flangeability of sheet metal can be evaluated by the hole expansion ratio (HER), which is defined according to the ISO 16630 standard [2]. The ECT is aimed to produce stretching conditions on thin sheets by imposing a hemispherical punch against a clamped specimen placed between a die and a blank-holder. The formability is measured by the punch displacement until the crack appears, also called the Erichsen cupping index (IE) by the ISO 20482 standard [3]. In this work, we developed a low-cost mechanical device capable of performing the HET and ECT tests using a universal testing machine. In order to verify its functionality, tests were carried out with the dual-phase steels DP600 and DP780. The corresponding values determined for HER and EI provided reliable results in terms of the accuracy and repeatability of the proposed testing device

Keywords— Hole expansion ratio; Erichsen cupping index; Dual-Phase steels.

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1) Sustainable Manufacturing Solutions
   a. Manufacturing Processes & Simulation

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Challenges and perspectives in additive manufacturing of ceramic materials: an overview of the mechanical properties in the alumina-zirconia system

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***Abstract*— Additive Manufacturing (AM) techniques have gained high representativeness on material processing as a substitute technology to conventional ones, providing new opportunities and conceptual freedom. Continuous development and innovation of these techniques is a current trend, and, in the coming decades, it is expected that a shift for AM processes will present a significant impact at both economic and social levels. Such effect will be reflected in the value chain of manufactured products, namely the equipment and supplier costs, as well as the value of professional services, including product engineering and design[1][2]. Concerning ceramics processing using Additive Manufacturing techniques, some are presenting promising results, for example, robocasting[3], lithography ceramic materials (LCM)[4], and selective laser sintering (SLS)[5]. In the present work, and based on a literature review, a map of the most significant mechanical properties of the 3D printed alumina-zirconia system, obtained by the most relevant AM technologies for ceramics, will be analysed. Alumina-zirconia system is widely used in several functional applications, due to their excellent mechanical behaviour, being currently materials of high interest in AM research field. When alumina and zirconia are compared, typically the first has high hardness and Young´s modulus, while the second present's high flexural strength and fracture toughness. In alumina-zirconia mixtures, specific compositions present unique characteristics, given focus to zirconia toughened alumina (ZTA)[6] that is a composite ceramic material comprising small zirconia grains (15 -30 vol%) in an alumina matrix. Another composite is alumina toughened zirconia (ATZ)[7] that comprises small alumina grains (15 -30 vol%) in a zirconia matrix, where the increase of the fracture toughness and consequently higher strength resistance is observed. Therefore, a map of the most significant mechanical properties of the 3D printed alumina-zirconia system, obtained by robocasting, LCM, and SLS will be analysed. In comparison to robocasting, LCM, and SLS, the mechanical properties of the 3D printing ceramic parts present distinct differences. In general, Robocasting and LCM exhibit better mechanical properties in comparison to SLS. Additionally, Robocasting is the AM process that offers better feasibility to obtain hollowed and multi-materials structures.**

Keywords*— *Additive Manufacturing; Advanced Technical Cermaics; Alumina-Zirconia System; Mechanical properties.

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Effect of ammonolysis temperature on physical properties of vanadium (oxynitride) as a potential electrocatalyst for ammonia decomposition

Synthesis, crystal structure and eletrical properties

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Abstract— **Ammonia (NH_3) is considered as a potential energy carrier to be used as a fuel in energy conversion devices, such as the solid oxide fuel cells (SOFCs). These eco-friendly systems can directly convert chemical energy into electricity. However, a key challenge still remains for finding alternative anode materials, aiming to improve the durability and the performance of the cell components. Hence, the present work is dedicated to the synthesis and characterization of vanadium oxynitride ($VO_{1-x}N_x$), as a potential novel earth-free anode material for NH_3-SOFC. The rock-salt structure (Fm3m) of $VO_{1-x}N_x$ can be simply formed when V_2O_5 reacts with gaseous NH_3 in the temperature range 600 – 1000 °C. X-ray diffraction and Rietveld refinement reveal that the unit cell volume increases with increasing the ammonolysis temperature, being concomitant with the increasing amount of nitrogen incorporated into the anionic sublattice measured by thermogravimetry. The use of lower ammonolysis temperatures is, therefore, beneficial to obtain small crystallite sizes, with increased lattice strain, as measured by Halder-Wagner method. The material exhibits very high electrical conductivity in reducing conditions (1120 S cm^{-1} at 800 °C), showing a slightly negative dependence (E_a = 0.04 eV) with temperature, which evidences its typical metallic behavior.**

Keywords— ammonia fuel, SOFC, vanadium (oxy)nitride.

ACKNOWLEGEMENTS

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Exploring NbN material as electrocatalyst for ammonia synthesis by ammonolysis route

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Abstract— **Interest in ammonia (NH3) synthesis research has been increasing over the past years due to its valuable application in many products. Ammonia is a chemical building block for the fabrication of plastics, explosives, pesticides, fertilizers, etc. Moreover, due to its very high energy density, it has also been considered as an alternative carbon-free fuel that can play a crucial role in a sustainable energy future. The current industrial process for NH3 synthesis is the Haber-Bosch process (HBP), however, this process is estimated to be responsible for 2.5 % of worldwide greenhouse-gas CO2 emissions. To solve this problem, research has been focusing on alternative fabrication technologies, where one of the most promising is the electrochemical synthesis of ammonia. However, one of the key limitations of the electrochemical ammonia synthesis is to find suitable catalysts for to break the nitrogen molecule. Transition metal nitrides ((TM)N) have been highlighted by DFT calculations to offer high catalytic activity for the ammonia formation reaction, whilst suppressing H2 evolution (HER) [1] , although experimental validation is currently lacking. Hence, in this work, we aim to study the synthesis and stability of niobium nitride as potential electrocatalyst for ammonia synthesis using X-ray diffraction and thermogravimetry.**

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This work is supported by the projects: SFRH/BD/130218/2017; PD/BDE/142837/2018; UID/EMS/00481/2019-FCT - FCT - Fundação para a Ciencia e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Program (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.

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Integrated Methodology for Designing ALM Structures

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***Abstract*— The potential of Additive Layer Manufacturing (ALM) is high, with a whole new set of manufacture parts with unseen complexity being offered. However, the process has limitations such as minimum member size or overhang constraint, which should be accounted in the design. Thus, the combination of Topology Optimization (TO) with ALM has been seen as an advantageous combination [1]. However, the transition between TO and ALM is a non-trivial step that requires a robust methodology. Thus, an integrated methodology is needed and, therefore, presented. The TO step is available and accounts for minimum member size (Heaviside projection) and/or overhang constraint (layer-wise simplified fabrication model) [2]. The algorithm uses a regular cube approach with precomputed stiffness matrices for efficient assembling and solving. The referred transition between TO and ALM is also available via Laplacian smoothing. The source code is available on GitHub in the Trimesh module and all the auxiliary tools are available, namely geometry import and export capabilities, visualization capabilities and interactive boundary conditions selection [3]. Finally, a 3D application is presented illustrating the integrated process.**

***Keywords*— *Topology optimization; Minimum member size; Overhang constraint; Laplacian smothing; Trimesh*.**

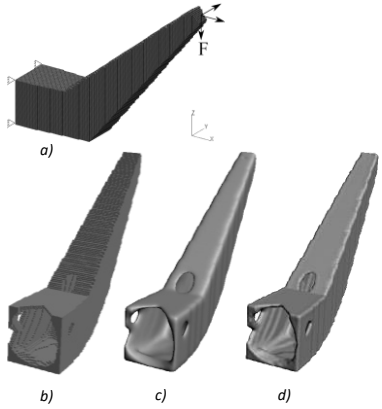

Figure 1- (a) Design volume and boundary conditions, (b) Topology Optimization, (c) Laplacian smoothing and (d) Taubin smoothing of the Sentinel-1 Antenna Support Bracket.

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The authors gratefully acknowledge the financial support of the Portuguese Foundation for Science and Technology (FCT) for the following projects (i) CENTRO-01-0145-FEDER-029713, (ii) CENTRO-01-0145-FEDER-022083, (iii) CENTRO-01-0247-FEDER-024039 and (iv) SFRH/BD/120779/2016 (B. Barroqueiro scholarship).

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   a. Manufacturing Processes & Simulation.

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Material Behaviour Models of Ti6Al4V Machining using Finite Element Analysis

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***Abstract*— Machining is a complex manufacturing process involving several physical phenomena, including large deformation of the workpiece material, complex friction conditions between the cutting edge and the workpiece, thermo-mechanical coupling between deformation and temperature fields and material failure (metal chip formation) [1, 2]. The described mechanisms are affected by the cutting conditions in which the process happens, therefore, modelling machining operations can be challenging.**
One way to modelling machining operations is by using experimental setups, in which the entrance and response variables are quantified and used in statistical modelling and analytical models. However, to achieve accurate results with experimentation, a high number of laboratorial tests is required [3].

Finite element method (FEM) can be a powerful tool to perform numerical simulations of machining operations (Fig 1.). The machining process response, in terms of cutting forces, tool and workpiece temperature, metal chip morphology, strain and strain rate can be evaluated since the cutting conditions (that happen in real machining processes) can be reproduced in those models. Consequently, FEM can be used as an intelligent tool to plan experimental tests in order to save time, reduce wasted material and cutting inserts [3].

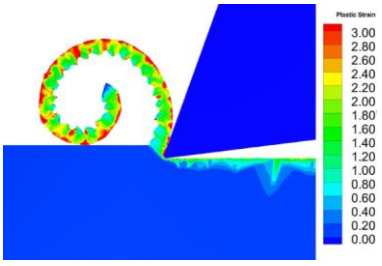

Figure 1- Numerical simulation in Orthogonal Cutting for Ti6Al4V alloy, metal chip, tool and workpiece are represented. The red color represent regions were a higher plastic strain was achieved.

The aim of this work was to model orthogonal cutting operations in Ti6Al4V Titanium alloy using a finite element analysis software called Third Wave AdvantEdge 7.501. Aspects regarding the development of machining simulations were explored, including different workpiece material behaviour models and the generated response variables, including the cutting forces and cutting temperature. Experimental setups from the literature were used to explore and validate models. The obtained results were helpful to understand the effect of the chosen workpiece material models and selected parameters in the process response variables.

Keywords*— *Finite Element Analysis; Machining; Ti6Al4V.

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Microwave Porcelain Firing

Material properties

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Abstract— **Porcelain manufacturing is highly energy consuming, natural gas being the most used primary energy source. Gas and electric heating are the conventional heating technologies, with heating cycles of the order of 200 min [1]. Faster heating originates thermal gradients in the pieces, leading to probable non-uniform properties and cracks formation [2].**
Microwave is presented as an alternative heating technology for porcelain firing [3,4]. The microwave furnace has a nominal heating power of 5.4 kW, provided by 6 magnetrons. As porcelain is a poor microwave absorber, the silicon carbide (SiC) plate that is the base for the porcelain samples is also a susceptor [3,4]. Porcelain starts receiving heat from the susceptor, and as its temperature rises it starts absorbing more and more microwave radiation. When controlled, microwave heating is volumetric, allowing higher heating rates without cracks formation [3,4].
Sets of 12 samples were fired from room temperature up to 1410 ºC when microwave fired, and up to 1475 ºC when electrically fired. Samples' temperature was measured by a pyrometer (surface) and by a backup thermocouple (neighboring).
Physical properties such as impact resistance, water absorption, apparent porosity, bulk and apparent densities and shrinkage were evaluated and analyzed. Microwave and electrically fired samples have equivalent properties, microwave firing requiring temperatures approximately 80 ºC lower than that required by the conventional firing (1380 °C) and 60% shorter processing times.
The lower temperatures required by microwave firing are not attributed to the non-thermal microwave phenomenon, but to the insufficient knowledge of the samples' temperature.
As porcelain has a poor thermal conductivity, the temperature inside the ceramic material is higher than at its surface when microwave fired, knowledge of their interior temperature remaining inaccessible. The capacity and the complexity of microwave firing, related with the materials dielectric and thermal properties, and the electromagnetic field distribution inside the furnace (samples), were simulated using COMSOL Multiphysics [3,5]. The knowledge of the electromagnetic field patterns and its dynamics helps to minimize the non-homogeneity of the electromagnetic field, minimizing temperature differences in microwave fired samples. This helps understanding of the properties differences between microwave and conventionally fired samples, and between microwave fired samples of the same batch.

Keywords— Porcelain; Microwave firing; Material properties.

ACKNOWLEGEMENTS

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Mode I fracture of hybrid NFRC

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***Abstract*— This paper describes hybrid natural fiber-reinforced composites (NFRC) that use different reinforcement fibers in their matrix. Hybridization is a technique used to improve the performance of the composites. Combining different fibers can meet the necessities of the application and results in a sustainable product [1]. The reason for studying this theme is the search for new materials that can replace traditional engineering materials, combining the lowest price, lightness, noncorrosive, and good mechanical strength, etc. Aeronautical, automotive, sports industries, etc., search for these materials, due to the advantages mentioned. Some applications are shin guards, helmets, door panels, dashboards, headliners, and seat backs, etc.**
The fibers used were Jute, Sisal and Curauá. They were chosen because they are available in large quantities in Brazil. In the research of NFRC's, there are many gaps, for example, mechanical and thermal characterization, and sensitivity to delamination. To obtain properties near the synthetic fiber-reinforced composites (e.g., glass fiber), which are aggressive to the environment, hybrid composites reinforced with vegetable fibers is an alternative in the replacement of synthetic fibers.
Thus, this work investigated the effects of hybridization on the fracture toughness and delamination of Sisal (S), Sisal+Curauá (S+C), Jute (J) and Jute+Curauá (J+C) epoxy composites. DCB tests were performed in Mode I loading according to ASTM D5528 standards [2]. The average values of the initial critical energy release rate from Mode I were calculated using three different data criteria, the deviation from linearity (NL), the 5% offset/maximum load (5%/Max) and visual observation (VIS) [2] [3]. It was shown by the experimental results that the hybridization process improved the values of the critical energy release rate from Mode I of the hybrid composites J+C and S+C when compared to the pure composite J and S to all different data criteria. To contribute, this work intended to show the importance of the hybrid composite studied, once natural fibers have a lower environmental impact, are sustainable, and present technical and economic feasibility in the search for innovative materials for engineering.

Keywords— Hybrid natural fiber reinforced composites; Delamination;DCB Mode I.

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Study of Improvement of an Aluminium Alloy used in the Aeronautical Industry

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***Abstract*—The aeronautics industry is increasingly investing in the development of new materials that meet the high-performance requirements of this area. These developments are associated with a pursuit for more economical solutions. This work studies the possibility of improvement of the AA6061 aluminium alloy through asymmetric rolling processes and heat treatments. The effect of the various types of rolling (conventional and asymmetric), as well as other parameters of this process, is explored. Previously recrystallized samples are subjected to different ratios of the roll's velocities (1, 3 and 1.36), thickness reduction per pass (20% and 50%) and forming routes (conventional, asymmetric continuous and asymmetric reverse). The mechanical properties and crystallographic texture of the samples were analyzed in order to correlate the results obtained with the different process conditions. Data were obtained through hardness and uniaxial tensile tests, and EBSD analysis. After rolling and annealing, significant increases in hardness were observed in the samples. All samples show a large increase of yield and ultimate tensile stress, while the formability drastically decreases, being more pronounced for sample processed with a 50% rate reduction of thickness. The EBSD analysis reveals a formation of copper {112} <111>, shear 1 {001}⟨110⟩ and shear 2 {111}⟨112⟩ texture components which explain the large increase in mechanical strength. It is concluded that the mechanical properties of this aluminium alloy can be enhanced originating strength values higher than the AA6061-T6 alloy. The limitations regarding the reduced material formability can be reviewed in the future by applying new heat treatments.**

Keywords*— *aeronautics, aluminium alloy, asymmetric rolling, mechanical response, crystallographic texture

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TOPIC

1) Sustainable Manufacturing Solutions
   a. Manufacturing Processes & Simulation

Understanding the Carbon Cycle: The Need for Carbon Sequestration

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***Abstract*— The current trend of global warming is undeniably linked to a build-up of CO_2 in the atmosphere due to heavy use of fossil fuels. Atmospheric CO_2 concentration is predicted to more than double by 2050, hitting levels not seen in 50 million years, unless we quickly intervene.[1] A solution must begin with an understanding of energy production and consumption and CO2 point source emissions.[2,3] Effective intervention requires deep understanding of the carbon cycle. There is a lot of misinformation. Planting more trees has been proposed as part of the solution. Plants are sustainable. They take care of themselves. However, over the whole life of their carbon cycle, they provide no net removal of CO_2. Trees pull CO_2 from the atmosphere to grow biomass via photosynthesis. However, when they die, they decompose, and release their carbon back to the atmosphere. Animals are fed plant biomass, and humans are fed plants and animals. They exhale CO_2 back to the atmosphere. They accumulate carbon during their lives but release their carbon when they die and decompose.**

The Kyoto Protocol adopted in 1997 and entered into force in 2005 committed industrialized countries to limit and reduce greenhouse gases emissions in accordance with agreed individual targets.[4] The U.S. responded by mandating the blending of bioethanol into gasoline. Europe went diesel. The U.S. produces bioethanol primarily from corn. To achieve the 10% ethanol in the U.S. gasoline pool, about 40% of the U.S. corn crop is now devoted to ethanol.[5] However, gasoline is only about 50% of refinery output, and transportation fuels are only about 30% of total primary energy needs.[2] The production of bioethanol will be examined in terms of the carbon cycle (not just the fate of carbon in the corn kernel feedstock and ethanol itself from the conversion of corn kernel starch, but also the fate of the rest of the plant).

While non-CO_2 emitting power generation from wind and solar energy will help, and has seen explosive growth, renewable sources are projected to account for only 10% of primary energy consumption out to 2035.[3] Fossil fuels will continue to supply the bulk of our energy needs.[6] The only way to stop future CO_2 emissions from fossil fuels is CO_2 sequestration. We know how to do it. It will just cost money, and scale-up is a major issue. The technologies for CO_2 sequestration will be reviewed.

While CO_2 sequestration will reduce future CO_2 emissions, it will not reduce the amount of CO_2 already in the atmosphere. The only way to do that is biomass carbon sequestration. Biomass grown from CO_2 in the atmosphere must be removed from the carbon cycle. Instead of putting capital and energy into converting biomass to biofuels processes, which are inherently inefficient, skip the middleman. Attention must be focused on biomass carbon sequestration.

Keywords*— *Global Warming, Carbon Cycle, Bioethanol, CO_2 Sequestration

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TECHNOLOGIES FOR THE WELL-BEING

Adaptive predictive control strategies of tankless hot water production

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Abstract— **Universally, a domestic potable water heating contributes between 15% and 40% of energy consumed within residential dwellings [1]. Among all trading technologies available, Gas Tankless Water Heaters (TGWH) are sold in large numbers and seen as an efficient means of domestic hot water production with a far smaller carbon [1]. However, its users comfort perception is severely affected by sudden water temperature changes away from the desired temperature [2]. The instability of the water production temperature with overshoots or undershoots is the most common drawback of gas tankless water heaters devices. This is mainly due to sudden changes on the overall water flow rate demand and the response delays inherent to the heating system, which can't be anticipated by the conventional embedded controllers [2]. Several advanced TGWH devices use a gas modulation, feedback flow rate, temperature sensors and PID controllers [3]. Furthermore, the studies [4] and [5] report that the most promise alternative solution is the model predictive control (MPC) for instantaneous electric water heaters. In addition, due to the dominant nonlinear dynamics in TGWH behavior, feedback control design becomes more difficult and then leads to performance drops [6]. Therefore, an adaptive predictive control strategy, technique that has attracted attention nowadays, was used in this research work combined with a TGWH dynamic model. Adaptive MPC provides a new linear model at each time step as the dynamic operating conditions change. Thus, it makes predictions more accurate for the following time step as compared with traditional MPC, which uses a constant internal model. The TGWH model under study was presented in detail by [2, 3, 7], and a virtual test bench is already available at the Thermal Laboratory. The virtual test bench is designed to be innovative and perform HIL simulations and allows for the incorporation of TGWH hardware within a software simulation, in particular, Matlab and Simulink environment is used in the present work. It can incorporate the real system, the real controller, typically a micro controller (µC) and the virtual simulation in real time. The investigation also takes into consideration the time delay, discretization and the linearization processes of the model. Besides the findings agreed well with the reference set-point, adaptive MPC presented closest results agreement against conventional MPC, in particular at flow rate changes regions. Finally, the ongoing research work is aiming to test the embedded control within the test bench in virtual and real control of TGWH.**

Keywords— tankless hot water production; predictive control strategies; adaptive control; virtual test bench; real time.

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Adsorption heat pumps

Towards modeling and simulation of the complete system

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Abstract— **Stopping global warming is one of the major challenges of our time. Development of heat pump technologies using refrigerants with very low or even null global warming potential (GWP) provides valuable contributions for that purpose. Adsorption heat pumps (AHPs) are one of these technologies since they work with natural refrigerants with zero or near zero GWP, commonly water, ammonia, ethanol or methanol. Unlike conventional vapor compression heat pumps, AHPs do not require electricity to circulate the refrigerant since they are driven by thermal energy, which can be acquired from waste heat, geothermal sources, solar collectors, gas burning or electric heating.**

Most recent advances in adsorption heat technologies are focused on the adsorbent-adsorbate working pair kinetics, heat exchanger designs and operating conditions. Moreover, detailed studies and numerical models are only applied to standalone adsorbers [1]. As reported in [2], in order to accurately describe the adsorber's dynamics, a distributed parameter model is required instead of a lumped one. Detailed models on the dynamics of adsorbers when integrated with the remaining system's components are not available in the literature. Such models provide major contributions to improve the AHP systems' design and performance.

An AHP system consists on the following major components: adsorber, evaporator, condenser, expansion valve, hot water reservoir and heat transfer fluid circuit. A detailed numerical model capable of describing the dynamics of the entire AHP system was developed. The physical model is described by a system of partial differential equations (PDEs), which are solved through a developed Matlab routine. The method of lines is used to transform the PDE system into an ordinary differential equations' system. Finite difference methods are implemented for the spatial discretization. The dynamic model can be used to perform sensitivity and parametric analyses of complete AHP systems with adsorber configurations consisting of an adsorbent material packed or coated around cylindrical tubes. This simulation tool outputs the time dependent pressure and temperature fields inside the adsorbent material, heat transfer fluid and hot water reservoir, as well as the mass of adsorbate adsorbed in the adsorbent material. The time evolution of these physical variables is of major relevance for the accurate estimation of the coefficient of performance (COP), specific heating power (SHP) and heating power (HP) of AHP systems. The obtained COPs are in the range of 1.2-1.5, which is in line with the experimentally obtained COPs reported in the literature.

The developed simulation tool provides detailed knowledge on complete AHP systems, which can be used to improve their design and performance. Results can be used for many purposes, like to analyze the performance of different working pairs, improve the adsorber's design, sharpen the control over AHP systems, tune the operating conditions, and give valuable information for the AHPs project design.

Keywords— Adsorption heat pump system; adsorption heat; dynamic model; numerical simulation; system's performance.

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Application of gain-scheduling MPC for domestic water heaters

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Abstract— **Presently there is a growing consciousness and concern with the scarceness of natural resources, associated with the noticeable increase in energy consumption and environmental harmful emissions. Domestic water heating is a major part of buildings energy consumption, where tankless gas water heaters (TGWH), also referred as gas-fired instantaneous, are extensively used. One of the most relevant drawbacks of TGWH is the difficulty of control the outlet hot water temperature as changes in hot water flow rate can be quick and unpredictable. These sudden changes of hot water demand, associated with the system inhered delays, origins temperatures overshoots and undershoots that severely affect the comfort perception by the user [1].**

One of the most promissory approaches to improve TGWH temperature stabilization is model predictive control (MPC). Advanced control strategies, such as MPC and adaptive techniques, can increase safety and comfort indicators by reducing water temperature undershoots and overshoots. As the best known by the authors, there aren't any successful implementations of adaptive predictive control in TGWH in the literature.

In a previous work [2], modelling and simulation of TGWH systems were performed, a lumped space approach was used to model individual components of the system, describing thermal, fluidic and mechanical dynamics. The system is described by a nonlinear semi-empirical model with input and output delays. The input delay is approximately constant and derives from the thermal power delivery process, the output delay is associated with the water travelling the pipes of the heat exchanger, is time-varying and inversely proportional to the water flow rate. The presence of time-delays imposes several difficulties and restrictions to the controller, particularly time-varying delays.

The development of MPC strategies for TGWH is particularly challenging, due to the limitations imposed by the need to embed the control on microcontrollers with limited computational and memory resources. In embedded MPC a convex quadratic problem is solved in each cycle, obtaining sub-optimal values limited to the execution time. In this work, a linear MPC design is employed for the stabilization of a constrained nonlinear process, however, control performance degrades significantly when operating far from the linearization operating point. The idea is to design multiple linear MPC controllers, each with its own linear state-space model describing process dynamics at a specific level of operation, with constant time delay. The active controller is selected based on the current state value and the measured disturbance of water flow rate, in a gain scheduling control strategy. This switching logic limits the on-line computational burden by transferring most of the computations off-line. Implementation details and preliminary results of embedded gain-scheduling MPC for TGWH are presented.

Keywords— tankless gas water heaters; domestic hot water; model predictive control; Embedded; gain-scheduling.

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Artificial Neural Network Modelling of Solar Thermal Hybrid Façade

Data Acquisition Setup and Data Gathering

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Abstract— **Climate change and sustainable development are some of the 21st century greater challenges. Renewable energies technology has reached a point where it becomes affordable to produce on-site the energy necessary to fulfill the needs. This producer-consumer paradigm can become a synonym of sustainability (supply-to-demand matching), energy efficiency (closer production and consumption means less energy transport losses) and security of supply (production is endogenous). It should be noted that the cost of renewable energy is becoming increasingly lower (the cost of energy obtained from renewable sources is easily calculated and relates to the return on investment made in the system and its maintenance) and the uncertainties in the fluctuation of energy costs have a low degree of instability and will depend mostly on the maintenance of the system. This approach leads to a better environment with less air and noise pollution resulting in greener cities. In this work it is intended to demonstrate the potential offered by a hybrid solar thermal façade which heats air and water, cools air and may also be used for passive ventilation. The façade can be used in several contexts, such as: industrial processes with lower enthalpy requirement, commercial buildings, hospital and hotels. The economic/financial analysis of the solution is a rather important factor that may decide the viability of such a façade in a determinate location. To provide such information a model of the façade will be created using an Artificial Neural Network (ANN). The use of artificial neural networks in various applications related with renewable energies, energy management in buildings and thermal systems analysis has been increasing significantly over the years [1]–[3]. This technique has, however, a different approach when compared with others as it uses and depends on data collected previously from a working prototype or a simulated system. This data should characterize the system behavior/performance during a rather large period and will be used afterwards to train the network which will then replicate the façade's working behavior. This paper intends to describe the equipment used for gathering data, the data acquisition setup/layout and to analyze some of the gathered data like air-flow, water-flow, fluid temperatures, sun irradiation, etc.**

Keywords— Artificial Neural Networks; System Modelling; Solar Thermal; Renewable Energy.

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Barriers to Increasing Wind Energy Contribution in to Islands Networks

(The case of Cape Verde)

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***Abstract*—This work intends to identify the main existing barriers in face of the increase of the contribution of the energy from the wind sources in the grid, taking as case studies the islands of Cape Verde. It is also intended to evaluate the quality of electricity in the network of the main island of the archipelago in reference -Santiago, with the aid of DIgSILENT Powerfactory 2018 software[1]. Thus, in the first stage of this work the wind market is analyzed, evaluating the evolution rate of the contribution of the wind resource in the energy matrices of the main markets, and then takes a critical look at the evolution of the island markets, focusing on the Cape Verde, where, despite the existence of an exceptional wind resource, only 10% of this resource is exploited, resulting in an average national network penetration of around 13% in 2018[2]. With the oil crisis that occurred in 1973, many countries are starting to bet on renewable technologies, but initially these technologies were quite expensive. For example, in 2008, installation costs for an onshore wind farm ranged from € 700 / kW to € 1000 / kW and offsohre was around € 1500 / kW[3]. Currently, modern onshore wind farms, depending on wind speed, can generate electricity at € 0.03 / kWh and € 0.08 / kWh and offshore parks can generate electricity between € 0.05 / kWh and € 0.08 / kWh[4]. Despite these significant advances and the existence of extraordinary wind potential worldwide, there are still major barriers that inhibit many countries from maximizing the contribution of wind energy to their energetic matrices. Among the many barriers identified are: public policies, financing and technical / operational aspects. Two main sources of risk can be associated with wind power production: (i) wind resource reliability and (ii) the use of wind power equipment[5]. It has been found from the simulation of the Santiago island power grid that harmonic voltage distortion increases with increasing wind generation capacity and therefore additional harmonic control means are usually required. This can be a barrier to the large increase in wind power on the grid as the costs of installing harmonic reduction techniques, such as synchronous converter installations, can be as high as 150% of the base value of the simple system.**

Keywords— Barriers; integration; wind; energy; grid.

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Connected and autonomous vehicles in mixed traffic flows: assessing energy and emissions potential benefits

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***Abstract*— With a predictable scenario of co-existence between connected and automated vehicles (CAVs) and conventional vehicles (CVs), this paper intends to explore potential effects of CAVs technology in reducing greenhouse gases (GHG) and pollutant emissions. Improved fuel economy and emissions reductions per unit of distance are expected from CAVs presence, mostly due to more gradual acceleration/deceleration patterns and fewer stop-and-go movements, as previous research has shown, while focusing on understanding how driving behaviour parameters affect infrastructure capacity, energy consumption and emissions [1].**
Although existing studies point that significant emission and fuel reductions could be obtained by introducing CAVs, little is known about how CAVs and CVs would co-exist and perform while a transitional period occurs [2]. Though, a microscale model platform for traffic and emission was applied in order to simulate a medium-sized city in European context, during the morning peak period. Four different road sections were selected (one motorway, one rural and two urban) which allowed to analyse in detail the impact of CAVs for each type and over different CAVs penetration scenarios. Considering different road types, this study is based on improved operational parameters (CFAP- Car Following Adjustment Parameters) [3] [4], assuming CAVs to behave like eco-driving agents to influence environmental impacts of traffic in general.
Observations could show that the impact may be positive, in terms of carbon dioxide (CO2) and nitrogen oxides (NOx) emissions, for certain types of roads, but may also be detrimental for congested traffic contexts. Particularly, results have shown that CAVs advantages are more pertinent in motorway (up to 30% reduction) and rural (up to 20%) sections, while in urban context the benefits kept a reduction of 7% in NOx emissions, comparing to baseline scenario.

Keywords — Connected and Automated Vehicle; Car following adjustment parameters; Vehicle specific power.

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Development of 4D structures for custom bolus production for external radiotherapy

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***Abstract*— External radiotherapy is one of the modalities used in cancer treatment. This technique involves the use of a beam of radiation that is directed at the tumor cells to destroy them and prevent their growth. Radiotherapy can be applied in two ways: external or brachytherapy. This work is dedicated to external radiotherapy, which is the choice when the tumor is most superficial and a radioactive source that is at a considerable distance from the tumor is used [1,2]. When the radiation beam interacts with the patient, it exhibits a certain behavior. Upon penetrating the skin, the beam deposits an amount of radiation dose that increases until it reaches the maximum point of depth. After this peak, the radiation dose decreases exponentially until it reaches the patient's exit point. In order for external radiotherapy to have better results, the maximum depth point must match the point where the tumor is located. Often in superficial tumors these two points do not coincide [2,3]. One way to solve this is to add a bolus to the external radiotherapy process. The bolus is a layer made of a material of varying thickness that will be placed over the surface of the skin to be irradiated, simulating the layers of human tissue, allowing that the radiation depth point matches the spot to be treated, without the air interference. In addition to assisting the superficialization portion of the maximum dose point, the bolus may also correct irregularities that the patient's surface may contain or replace missing tissue [4,5]. 4D printing allows the creation of an object through 3D printing that, when exposed to a particular stimulus, changes its shape in a controlled manner. By using this technique, it is possible to reduce printing costs while making the most of its potential to develop devices with complex and adjustable structures, important features in this study, given the goal of creating custom patient structures. Post-print shape change is achieved by the correct selection and combination of materials and filament structure in the 3D printing process, coupled with a stimulus. The stimulus may arise from interaction with solvents, thermal stimulation, pH changes, light induction, among other forms [6,7]. The main objective of this work is to use the 4D printing technique in the development of structures that can be used as a bolus for external radiotherapy.**

Keywords— external radiotherapy; bolus; 4D printing; shape memory.

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Electrospraying of primary chondrocytes for cartilage repair

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Abstract— **Electrospun scaffolds have long been used for cartilage repair, due to the topographic similarity between the electrospun fibers and the collagen fibers of the extracellular matrix (ECM) in the native cartilage. Still, while their nanotophography can be beneficial for the cell proliferative and spreading behavior, it greatly reduces the inter-fiber pore size, hindering cell migration and relegating tissue formation to the surface of the scaffold [1]. A possible solution for this structural limitation would be the direct incorporation of cells into the fibers during electrospinning of the fibrous scaffold, overcoming the challenges of cell infiltration into small pore sizes by literally surrounding cells with the fiber matrix as it is produced [1]. This can be achieved using cell electrospraying, a concept first introduced in 2005 by Jayasinghe, enables the deposition of living cells onto specific targets by exposing the cell suspension to an external high intensity electric field [2]. Cell exposure to the electric field, as well as the shear stress of passing through the cell electrospraying apparatus may affect cell viability and function, so several types of cells have been electrosprayed, and no significant influence was observed on a genetic, genomic and physiological level [4]. In fact, our previous work has demonstrated this inertness from a chondrocyte cell line (C28-I2) [5]. Still, these immortalized cells are genetically modified, and might not not accurately replicate the physiological conditions. Primary chondrocytes possess little proliferative ability, showing considerable dedifferentiation from a chondrocyte-like to a more fibroblast-like phenotype over time, particularly if growth factors are not used [5].**

In this regard, electrospraying experiments were performed with primary chondrocytes to assess the process influence on chondrocyte viability. After 24 hour-incubation, chondrocyte metabolic activity was measured, and these electrosprayed (E) cells were then slip and cultured in well plates and in three-dimensional anisotropic fibrous/porous scaffolds under static and perfused conditions. Non-electrosprayed (NE) cells were considered for comparison.

The obtained results confirmed that the behaviour of primary chondrocytes upon electric field exposure was significantly different from that obtained for the chondrocyte cell line, which can be attributed to the lower recovery ability of these cells. Nonetheless, an increasing proliferation rate was observed over time. The proliferation performance of NE and E primary chondrocytes on 3D environment followed a similar trend, with E primary chondrocytes possessing a significantly lower viability than the NE primary chondrocytes. The application of perfused conditions to the E chondrocyte-seeded scaffolds greatly increased the chondrocyte viability to values similar to the ones obtained for NE chondrocyte-seeded scaffolds. Even though the electrosprayed primary chondrocytes suffered a substantial proliferative delay, they were able to recover, particularly under perfused conditions, suggesting that these conditions should be implemented after the electrospraying process, so that this technology might become an effective approach to uniformly incorporate primary chondrocytes into electrospun scaffolds.

Keywords— cartilage tissue engineering, chondrocyte, electrospraying.

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Energetic optimization analysis of maintenance-free electric hot water production and storage systems

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Abstract— **The present work addresses an energetic and economic analysis of an electric hot-water storage (EWS) systems integrated with phase change materials (PCMs). In the first part, the transient behavior of a reference EWS, for which no PCMs was considered by resorting to the TRNSYS software. The second part addressed the incorporation of PCMs into the reference model by development of a full thermal dynamic numerical analysis. There is a considerable body of literature addressing the issue of modeling the behavior of PCMs at latent heat storage media within fluid heat tanks, particularly for residential EWS solar systems' applications restoring to the TRNSYS software. Some studies [1, 2] have been conducted an experimental solar pilot plant to test the PCMs behavior in real conditions employing granular PCM–graphite compound. Stratification effects were taken into account and the simulation was conducted with TRNSYS. The studies reported that adding a PCM module would give the system a higher storage density while compensating for the heat loss in the top layer [3]. In this work, a numerical solution has been developed by restoring to discretization with a predetermined number of non-overlapping control volumes for which each height position corresponds to a spatial node. The finite control volume method with a linear interpolation was used to discretize the mathematical governing equation, and a solution was obtained for the approximate form of the Navier-Stokes equations using a time implicit scheme to prevent stability limitations. The numerical model is capable of describing the behavior of a particular type of Thermal Energy System (TES) considering the time-dependent outlet temperature. The model employs a set of governing equations which economically and accurately characterize the dominant energy transfer mechanisms in the charging/discharging periods. The model was designed so that it could be applied to different configurations and sizes. The model was encoded within the FORTRAN environment, which allows compiling within energy simulation tools, namely, the TRNSYS - TypeStudio compiler creating a new TRNSYS' type that can be incorporated with weather files, controllers, pumps, power resources, bypass sachems, solar design etc. in the TRNSYS environment. The model can be used both for specific periods of time or for a more general analysis which includes system response over one-year periods. Simulation results include, but are not restricted to dynamic temperature response, performance, efficiency, energy consumption and allow economic approaches. The preliminary results for the identification of interesting system features. The ongoing research effort includes improvements of the numerical schemes, validation and optimization.**

Keywords— thermal energy storage; numerucal modeling; domestic hot water production.

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Fabrication of a 3D combinatorial fibrous-porous scaffold for neural tissue engineering applications

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Abstract— **The ability of tissue engineered scaffolds to modulate the response of neural stem cells (e.g. adhesion, proliferation and differentiation) is boosting the unlocking of advanced therapeutic strategies capable of attenuating the effects of traumatic pathologies like spinal cord injury [1]. From the wide range of reported scaffolding concepts, it has been consistently demonstrated that nanofibrous networks and graphene-based porous systems are proficient for guiding neurite outgrowth and inducing specific differentiation patterns, respectively [2].**

Following this trend, we propose a scaffold with a combinatorial fibrous-porous architecture with the final goal of recreating an *in vitro* 3D cellular microenvironment suitable to promote a noticeable impact in the viability and differentiation of the cultured embryonic neural progenitor cells (ENPCs). Briefly, electrospinning was used to fabricate biocompatible polycaprolactone-gelatin (PCL-gelatin) nanofibres with diameter of 200 nm. Such electrospun mesh was then accurately cut into small pieces and mixed into a reduced graphene oxide (rGO) aqueous solution with the intent of generating a hydrogel-like structure. Finally, it was possible to accommodate the nanofibres onto the surface of a 3D rGO microporous network after a controlled lyophilization process. Results showed that as the PCL-gelatin nanofibres covered uniformly the surface of the rGO sheets, the mechanical integrity of the scaffold was reinforced without compromising its 3D interconnected porosity and water uptake capability. Additionally, these complementary morphological features were responsible for inducing synergistic functionalities since the ENPCs were able to adhere onto the surface of the scaffold and efficiently differentiate into viable neuronal and glial cell types. In this way, during 14 days in cell culture, the biochemical and topographical cues provided by the fibrous-porous geometry were capable of stimulating neurite outgrowth and elongation through the scaffold, leading, consequently, to the formation of an interconnected neural network.

Taking this into account, the reported scaffolding approach presents potential not only to support therapeutic neural regenerative applications, but also to contribute to a better understanding of key factors related to the repair of the central nervous system after injury.

Keywords— Neural tissue engineering; Fibrous-porous scaffold; Electrospinning; Polycaprolactone; Reduced graphene oxide.

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Fabrication of electrospun scaffolds with cell laden hydrogel for cartilage tissue engineering

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Abstract— **Tissue engineering strategies create artificial substitutes for the regeneration of damaged tissues, beginning with the fabrication of scaffolds moving then to cell incorporation onto those scaffolds and subsequent tissue growth in vitro. Cell seeding techniques, unfortunately, are usually ineffective to develop scaffolds with homogenous cell distribution, resulting in non-functional tissue formation [1]. With electrospun scaffolds, cell incorporation becomes even more challenging. Electrospun scaffolds are a very tightly packed layer of fibers with small pores, that makes difficult the migration of cells onto the scaffolds, as well as, the diffusion of nutrients and wastes. To overcome this drawback, the direct incorporation of cells, using electrospraying technique, onto the scaffolds during the electrospinning process has been reported. Cell electrospraying is a jet-based technique that allows the spray of living cells onto the materials by applying an electric charge in a cellular suspension [2]. Several studies have proved that cells can survive and proliferate after electrospraying process [3], [4]. Still, previous work has shown that while uniformly distributed cell-laden scaffolds can be fabricated using this technique, some issues remain. Cell desiccation on top of the fibers due to longer duration of the experiment and inadequate cell environment – low temperature and CO2 concentration – and solvent toxicity are the main limitations for the optimal efficiency of cell electrospray process onto electrospun fibers.**

In this regard, in this work, the production of electrospun scaffolds was combined with the electrospray of chondrocyte laden hydrogel creating a shield/protection around the cells during and after the electrospray process, preventing its dehydration. For that, a polymeric solution of polycaprolactone (PCL) and gelatin was electrospun alternately with a chondrocyte-laden sodium alginate hydrogel electrospray. Sodium alginate is a natural polymer widely used in biomedical engineering due to its biocompatibility, biodegradability and ability to form hydrogels [5]. The prepared scaffolds were then cultured for 7 days and the respective cell viability assessed. The percentage of viability was calculated as a ratio of the metabolic activity of the electrosprayed chondrocytes and the metabolic activity of chondrocytes that did not underwent any process. The chondrocyte distribution was also evaluated.

On the first day of culture, the results showed that the cellular viability was higher than the one previous reported, demonstrating that the alginate hydrogel allowed the cells to survive and helps in its attachment. After 7 days of culture, cells continue alive with considerable viability increasing. It was also shown that it was possible to incorporate cells homogenously distributed by electrospraying process using the chondrocyte laden hydrogel. These results emphasize the potential value that the hydrogels can have on the electrospraying process with the electrospun scaffolds.

Keywords— Cell laden hydrogel; Electrospun scaffolds; Cartilage tissue engineering.

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Fin-and-Tube CO_2 Evaporators

Modelling, testing and validation under different hygrothermal conditions

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Abstract — Fin-and-tube heat exchangers are one of the major components of air-conditioning, refrigeration and air-source heat pump systems. When used as evaporators and exposed to moist airflows, their extended external surfaces are frequently below the dew point temperature triggering, at the airside, simultaneous heat and mass transfers. Determination of the cooling and dehumidifying characteristics is essential to the design and optimization of these heat exchangers and improvement of their operation, to enhance the overall system's performance. The appropriate design will not only reduce the evaporator's volume but also significantly reduces the refrigerant charge within the system. Furthermore, less bulky evaporators with smaller diameter tubes or channels, commonly used in CO2 vapor compression systems, tend to bring stratified type flow regimes into the annular flow, increasing the wetted perimeter used in the boiling process, enhancing the evaporator's performance.

This paper deals with the development, testing and validation of a numerical model for CO2 fin-and-tube evaporators operating under different hygrothermal conditions. The numerical solution is obtained through a MATLAB implemented finite volume scheme, using two different approaches based on the logarithmic mean enthalpy difference method. The first, the most referenced approach in the open literature, considers fully dry and fully wet surface conditions and unit Lewis factor [1]. Besides the first two conditions, the second approach also considers partially wet conditions and non-unitary Lewis factor [1], allowing consideration of the relevant effect of relative humidity on the mass transfer under such conditions. Although being more accurate, this approach requires the implementation of the finite circular fin method and a supplementary iterative process for determining the partially wet fin efficiency, demanding additional computational time. To the authors' knowledge, this approach has never been applied to natural refrigerants. On the refrigerant side, flow pattern based phenomenological models and maps were used. On the airside, different heat and mass transfer correlations, in Colburn j factors' form, can be used according to the evaporator's geometric features.

Although the existence of some stand-alone simulation software for fin-and-tube heat exchangers, found in the literature and available on the web, the proposed model provides its integration in a whole-system simulation tool. Once connected to other components models, such as compressor, expansion valve and gas cooler [2], its thermal performance can be evaluated, as well as its subsequent impact on the overall system's energy performance, providing relevant information for the design of efficient systems. Additional features provide an evaluation of the effect of airflow maldistribution profiles, arbitrary tube circuitries and different coil configurations.

Keywords — Fin-and-tube evaporator; CO2; numerical model; logarithmic mean enthalpy difference method; energy performance.

ACKNOWLEGEMENTS

The authors acknowledge the Portuguese Foundation for Science and Technology (FCT) for the financial support provided through the grant SFRH/BD/148378/2019 and the project UID/EMS/00481/2013-FCT, and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Program (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund. The present study was developed in the scope of the Smart Green Homes Project [POCI-01-0247-FEDER-007678], a co-promotion between Bosch Termotecnologia S.A. and the University of Aveiro. It is financed by Portugal 2020 under the Competitiveness and Internationalization Operational Program, and by the European Regional Development Fund.

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Impacts of Driving Volatility on Road Safety and Emissions: The DICA-VE Project

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Abstract— The main objective of this communication is to present the project "DICA-VE: Driving Information in a Connected and Autonomous Vehicle Environment: Impacts on Safety and Emissions", which aims to develop an integrated methodology to assess driving behavior volatility and develop warnings to reduce road conflicts and pollutants emissions in a vehicle environment.
A particular attention is being given to the interaction of motor vehicles with vulnerable road users (pedestrians and cyclists) [1, 2]. The essence of assessing driving volatility aims the capture of the existence of strong accelerations and aggressive maneuvers [3]. Alerts and warnings can enable calmer driving, reduce volatility and potentially improve road safety, traffic flow performance, fuel consumption and emissions. A fundamental understanding of instantaneous driving decisions, distinguishing normal from anomalous ones, is needed to develop a framework for optimizing road transportation impacts.
Thus, the research questions are: 1) Which strategies are adopted by each driver when he/she performs short-term driving decisions and how can these intentions be mapped, in a certain road network?; 2) How is driver's volatility affected by the proximity of other road users, namely pedestrians or cyclists?; 3) How can driving volatility information be integrated into a platform to alert road users about potential dangers in the road infrastructure and prevent the occurrence of crash situations?; 4) How can anomalous driving variability be reduced in autonomous cars, in order to prevent road crashes and have a performance with a minimum degree of emissions?
The specific deliverables of this project will be: 1) a complete and micro characterization of individual driver decision mechanisms; 2) a prototype of a driver warning and control assist mechanism to be applicable in connected or autonomous vehicles.

Keywords— Driving behavior; volatility; road safety; emissions.

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Integration of Machine Learning and Multi-Objective Optimization to Reduce Energy-Related Cost and Improve Thermal Comfort in Residential Buildings

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Abstract— **In order to materialize the interdisciplinary concept of intelligent supervised predictive control (ISPC) in the specific context of a residential building, this work integrated machine learning (ML) algorithm with a multi-objective optimization methodology to satisfy two opposing objectives. These objectives were defined such that to reduce human footprints on the environment without sacrificing their comfort which is also known as energy management. This is a non-destructive retrofitting procedure that can be applied to both new and existing buildings and with any level of HVAC technology.**
In this paper, the ML, as an application of artificial intelligence (AI), was employed to provide the air-conditioning control system with the ability to automatically learn and improve from experience without being explicitly programmed and without human intervention nor assistance. This paper focuses on the development of computer programs which can access data from weather forecast as well as embedded sensors and use them to learn how a given residential building should react to balance internal/external heat load with minimum energy consumption. Mitigation of energy consumption as well as enhancement of occupant's thermal comfort is our sought targets. Particle swarm optimization (PSO) was employed to find the global optimum of design variables. This stochastic optimization methodology is suitable for multi-objective, high dimensional, non-convex, non-continuous problems. After formulating the meta-objective function by combining two objectives through a weighted sum, an iterative procedure is carried out and a PSO routine tries to produce a new generation of design variables, which are more probable to result in a better meta-objective value. The thermal comfort of the occupants is measured by the Fanger's approach. A comprehensive modular code is developed to tune both heating and cooling set-points of the HVAC system. One important feature of this work is that only two free software has been employed for thermal simulation of building envelope as well as for ML and PSO functionalities. EnergyPlus (EP) was employed as the energy-simulator engine. Its capabilities include integrated simulation, combined heat and mass transfer balance, multizone air flow, HVAC loops etc. The EP, ML and PSO were integrated into a single code, written in Python language. In addition, the NN trainning, is made using data of the current timestep together with data of previous and later timesteps. This is an important feature since the thermal response of building, i.e. total energy consumption (TEC) and predicted percentage of dissatisfaction (PPD), highly depends on the building history. Moreover, weather conditions (outdoor temperature, outdoor humidity ratio), occupants' pattern and heating and cooling setpoints were considered as input data while TEC and PPD were considered as output data (building response).
The proposed supervisory predictive control can deliver robust, energy- and cost-effective decision, while being independent of the HVAC system.

Keywords— Intelligent supervised predictive control; Smart green home; Artificial intelligence, Machine learning; Particle swarm optimization.

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The present study was developed in the scope of the Smart Green Homes Project [POCI-01-0247-FEDER-007678], a co-promotion between Bosch Termotecnologia S.A. and the University of Aveiro. It is financed by Portugal 2020 under the Competitiveness and Internationalization Operational Program and by the European Regional Development Fund. Moreover, this work is supported by the projects: UID/EMS/00481/2019-FCT - FCT - Fundação para a Ciencia e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Program (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.

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NeuroStimSpinal

(A step forward to spinal cord injury repair using innovative stimulated nanoengineered scaffolds – FETOPEN No 829060)

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***Abstract*— The main focus of this project is the spinal cord injury (SCI), which is a devastating pathology with dramatic lifetime consequences affecting thousands of people worldwide. Therefore, and considering the very limited regeneration ability of the central nervous system, in this project we propose to develop a neural tissue engineered scaffold capable of not only combining fibrous and porous topographic cues in order to mimic the morphology of the native spinal cord (Figure 1).**

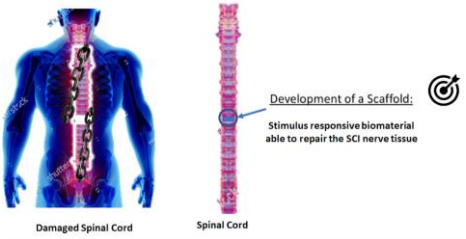

Figure 1- Proposed objective.

The radically new science-enabled technology that shall be developed in NeuroStimSpinal consists in an innovative stimulus-responsive cell-laden biomaterial able to repair the SCI nervous tissue. The proposed innovative biomaterial characteristic is a scaffold for implantation in the traumatic injury point composed of graphene-based materials (GBM) and human adipose derived decellularized tissue (adECM) to promote the growth and reconnection of the ruptured nerves (Figure 2).
The proposed innovation is based on a novel adECM/GBM hybrid composition. The adECM obtained by the partner TECNALIA demonstrated at TRL4: 1) Preservation of basal membrane proteins which play a role as passive molecular filtration and lead to a remarkable positive effect on cell differentiation and tissue repair; 2) Viability preservation of more than 139 proteins and 5 types of collagens, some of them with proven interest in neural regeneration; 3) Preservation of cell viability according to ISO 10993-5 with residual DNA amount. Preliminary studies by University of Aveiro partner has demonstrated that the presence of GBM in scaffolds further help the regeneration of neurons since these nanomaterials stimulate the ENCPs. A rupture point from similar approaches for this group is that the GBM based fibrous network will be placed in a oriented configuration instead of randomly dispersed, leading to a better stimulation of the SC structure and also beneficial cellular responses.

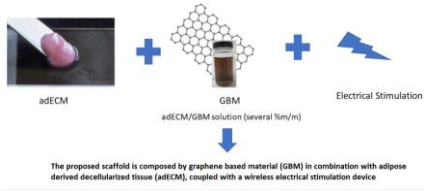

Figure 2- Scaffold design concept.

The foundational character of this project is to obtain a successful scaffold that promote the neural regeneration, axon growth and neural connection will establish an essential basis for a new line of scientific research in the neurological field.
The methodology to be followed includes; 1) Formulation of different adECM/GBM compositions, shapes and porosity matrices rationally designed for different SCI locations; 2) - Assess the biocompatibility, bio-functionality, performance (including electrical stimulation) of adECM/GBM scaffolds using embryonic neural progenitor cells (ENCPs); 3) Evaluate the systemic and long-term efficacy of cell-laden and non-cell-laden scaffolds with and without electrical stimulation using rat and rabbit in vivo models.

www.neurostimspina.eu

Keywords— FETOPEN; NeuroStimSpinal; Spinal Cord Injury; Graphene based materials.

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Numerical modeling Phase Change Materials for cold storage at chest freezers' evaporator coil

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***Abstract*— It is estimated that currently, energy consumption with refrigeration represents about 30% of the total energy consumed in the world [1]. Particularly, the use of refrigerators and freezers, is a source of large electricity consumption since today almost every home has at least one cooling system [2]. Food preservation is one of the main principles for wellbeing and quality in human life. Simultaneously, renewable sources of energy are in the front line for the climate change challenge.**

Vapor compression refrigeration cycle is commonly used on refrigeration systems and the energy efficiency enhancement has been developed on increased performance of heat exchangers, i.e., condenser and evaporator [3][4].

Particularly when talking about solid-liquid transition, phase change materials (PCMs) can store big amounts of thermal energy as latent heat so, they are one of the ways to achieve thermal energy storage when compressor is running. Hence, recent work on autonomy extension and energy efficiency enhancement emerged. By using PCMs some authors observed COP improvements between 5 and 15 % as well as extension of autonomy in 4 to 6 hours or even around 8% of energy savings when studying their impact on defrost cycles and door opening tests, for example [5][6][7].

The aim of the current study is to develop 2D numerical models using ANSYS-Fluent, regarding the use of phase change materials which melting temperature is negative. The idea is to analyze what happens to the material under different geometrical configurations and under different boundary conditions. This aspect is constrained by the final application on chest freezers' evaporator coils. Besides the results obtained by referenced researchers is highly important to do parametric studies on the influence of each thermal-physical property of the PCM in study for the final profiles of liquid-solid interface/profile and change phase temperatures and time needed.

From early simulations of a PCM around evaporator coil, Figure 1 elucidates on parametric studies available with this tool.

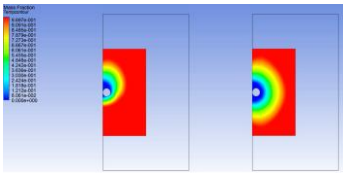

Figure 1- Liquid-solid interface evolution with different viscosity (Left<Right).

***Keywords*— phase change materials; cold storage; ANSYS Fluent; numerical modeling.**

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Optimizing Solar Photovoltaic Energy Capture and Storage Using Household Cold Appliances

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Abstract— It is estimated that there are about 1.4 billion home refrigerators and freezers worldwide. Their average individual consumption is about 450kWh/year. This amounts to about 14% of all residential consumption and an annual emission of 450 million metric tons of CO2 [1].

We will present new developments – both physical (i.e., hardware) and algorithmic (i.e., firmware) – towards the optimization of the capture and storage of solar photovoltaic (PV) energy using domestic freezers. This work was done in the scope of an ongoing research project in collaboration with industry, with the objective of developing an efficient consumer freezer appliance with extended autonomy, achieved through the use of Phase-Change Materials (PCMs) for Thermal Energy Storage (TES). This extended autonomy allows for such applications as: directly powering from a solar PV array and intelligent Load Management (LM) – e.g., relegating the work of the refrigeration machine to the periods of lower energy cost/demand [2] and/or of more efficient operation (i.e., colder ambient temperatures, e.g., at night). The freezer appliance is equipped with a variable speed compressor, whose modulation allows for the optimization of solar energy capture. The use of PCMs in the place of electrochemical batteries can lower the cost of the equipment considerably[3]–[5]. Notwithstanding, we will demonstrate that both options can be synergistically combined – through intelligent control – to increase the systemic efficacy and/or efficiency.

This type of research is increasingly relevant in the current global context, in which the push for decreasing CO2 emissions stimulates the investment in innovative technologies for increasing the efficiency in energy use, as well as motivating the growing share of renewable sources (e.g., mainly wind and solar) in the international energy markets. This increasing penetration of renewables is being capped by the difficulties that their lack of consistency and synchronicity between production and demand is causing in the management of an aging power grid infrastructure. In this conjuncture, the technological possibility of controlling the grid from the demand side is becoming inevitable, giving birth to the concept of the "smart grid". Control from the demand side is being achieved with the active participation of large energy consumers (mainly industrial). However, some household appliances offer an opportunity for including small consumers in a more comprehensive and, ultimately, more effective solution. These appliances consist of, mainly, thermal devices like water and space heaters, air conditioning units and, of course, the ubiquitous refrigerators and freezers.

Keywords— Solar Photovoltaic (PV); Domestic Refrigeration; Energy Efficiency; Load Demand Management; Smart Grids; Phase-Change Materials (PCMs); Thermal Energy Storage (TES); Electrical Load Management (LM); Direct Load Control (DLC); Home Automation (HA); Price-based Demand Response (PBDR).

ACKNOWLEGEMENTS

This work is supported by the project *«UFA+EE – Investigação e Desenvolvimento de Unidades de Frio Autónomas e Energeticamente Eficientes»* (Research and Development of Autonomous and Energy Efficient Cold Units), financed by the European Union through its Structural and Investment Funds, and through the programs "*Portugal 2020*", *"Programa Interface", "Sistema de Incentivos à Investigação e Desenvolvimento Tecnológico (SI I&DT)"* (System of Incentives for Research and Technological Development) with the reference *03/SI/2017.*

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PCM in thermal energy storage – a CFD approach

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***Abstract*— The use of renewable energy has been steadily rising over the years, with efforts to reduce emissions reinforcing this trend. However, renewable energy production is intermittent and a bridge over production/demand gap is required [1], with energy storage becoming increasingly needed. For thermal energy storage (TES), Phase Change Materials (PCM) represent a safe and inexpensive technique to match solar or residual heat availability to thermal requirements [2], [3]. One of the main questions regarding the use of these materials is how their thermal storage capacity of PCMs is affected by the low thermal conductivity of these materials, limiting the quantity of heat which can be stored or released during a given time interval. This attribute limits the response time of the heat transfer for these systems, as low heat transfer coefficient can lead to low energy transfer if the system is not properly designed [4]. Scientific developments in the subject are generally focused in the improvement of the heat transfer surface area, with reduced emphasis on methodologies that analyze the overall performance of PCM embedded TES systems, and the impact of changes to PCM usage in the transient behavior of those systems. While several advances in heat transfer and heat density of PCMs are visible in literature, the impact of these approaches in the behavior of these systems is still somewhat unclear. Both the heat transfer coefficient and the total energy stored are vital for the optimization of systems that include PCMs, and as such a deeper analysis of its interaction is required. In order to better understand this interaction a numerical model is being developed to study the influence of the convection heat transfer present during the charging and discharging phases by studying a base model using methods that fully model convection versus models that approximate that heat transfer to a conduction problem. This information is important for the development of a tool that enables the transient analysis of PCM embedded TES systems that will enable an in-depth analysis of the interactions between transfer coefficient and heat density.**

***Keywords*— Phase Change Materials; Numerical model; CFD.**

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The present study was developed in the scope of the Smart Green Homes Project [POCI-01-0247-FEDER-007678], a co-promotion between Bosch Termotecnologia S.A. and the University of Aveiro. It is financed by Portugal 2020 under the Competitiveness and Internationalization Operational Program, and by the European Regional Development Fund.

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Road traffic noise evaluation in urban areas

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Abstract— **Noise pollution due to road traffic is one of the most considerable issues in Europe. In fact, the damages for human health could go from the simple annoyance to sleep disorders, concentration deficit, up to cardiovascular diseases, and deafness [1]. The European Environment Agency estimated that 120 million of people in Europe are exposed to day-evening-night level exceeding 55 dBA while more than 50 million to levels higher than 65 dBA [2]. Moreover, the Organization for Economic Co-operation and Development asserts that emissions of air pollutants, carbon dioxide and noise produced by transport sector have a strong impact on the environment [3].**

There are two main ways to reduce the road traffic noise [1]: the first one acts directly on the source, leading to engine, tyres and road surface improvements; the second one provides the exposure reduction of people on the noise using insulation measures. Hence, the evaluation of noise in the critical areas is a matter of concern and could be performed in different ways, such as applying noise models or conducting measurement campaigns.

The noise models can be divided into statistical and dynamic. The first ones use only the distance between source and receiver and road traffic information to compute the relative noise parameter [4]. The second ones use kinetic information of road traffic flow as well as correction terms for driving state and road gradient [5].

One challenge in environmental noise monitoring is how to perform enough measurements both in time domain and spatially. This require costly equipment, large number of human resources and long periods of data collecting in order to capture the variability of road traffic operations.

Thus, the use of noise sensors as a way of collecting noise data shows as efficient in reducing monitoring-related costs in noise analysis. However, the evaluation of reliability of sensor measurements is a matter of interest fundamental inasmuch those data could be used as input for the implementation of new noise models, to create noise maps, monitor steadily the noise levels in cities critical hotspots and allow to plan corrective actions. Also, the installation of noise sensors often fails the phonometric rules, namely: 1) right orientation of microphone towards sources; 2) appropriate distance from reflective building and vegetation; and 3) impossibility to filter out data from strange events.

This work evaluated the reliability of sensor measurements by comparing with measured values. A total of 7 sensors installed in the city of Porto (Porto) were analyzed. The noise data are constantly recorded by them and, each five minutes the equivalent continuous sound pressure level is computed. The data given by those sensors were then compared with the recorded ones by a sound level meter in different periods of the day.

Results showed average differences between two instruments of 1.7 dBA. Although the goodness of the sensors was demonstrated, future improvements are needed to align them to phonometric rules, when the installation constrains allow it, in order to not compromise the validity of measurements.

Keywords— Road traffic, noise models, noise pollution, noise sensors.

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TOPIC

2) Technologies for the Wellbeing
   b) Innovative Technologies for Smart Cities.

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Simulation of photodegradation of nitric oxides at indoor levels using CFD

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Abstract — **Indoor air quality (IAQ) is a matter of a great deal of concern for public health. IAQ is influenced by a significant number of harmful substances including gases (carbon monoxide, ozone, radon, nitride oxides), volatile organic compounds (VOCs), other contaminants of organic and inorganic origin as well as bacteria, fungi, and pollen. These microscopic pollutants can penetrate deep into our respiratory and circulatory systems causing a lot of damage [1]. Unfortunately, conventional air filtration systems are not fit to deal efficiently with the destruction/removal of some of the above-mentioned contaminants. A technology based on principle of heterogeneous photocatalysis, earlier used for water purification and, has been applied in the recent years for indoor air purification especially in what concerns the degradation of VOCs [2, 3]and several harmful gases including but not limiting to nitrogen oxides (NO_x) [4, 5]. The encouraging results of the numerous applications of the Photocatalytic Oxidation (PCO) process for indoor air purification motivated investigation and development of novel and more efficient photocatalytic materials accompanied by an equal concern for improvement of numerical simulation methodologies of the PCO process. In view of the above, the objective of this study was the development of the numerical methodology for simulation of the NOx photocatalytic oxidation kinetics with special focus on improvement of its precision. Based on the experimental data, the reaction rates for different concentrations of NO_x at indoor concentrations levels (ppb) for two photocatalytic TiO_2 based materials were calculated by applying the Langmuir-Hinshelwood (LH) model described by its kinetic parameters, namely the Langmuir adsorption constant and reaction rate constant. To model the heterogeneous surface reaction, the sink term (representative of the surface heterogeneous reaction) was incorporated into a User Defined Function (UDF) and assigned to the respective photocatalytic surface. The results of the PCO simulations with the kinetic parameters calculated from the experimental data underpredicted the NO_x conversion at the outlet of the reactor for more than 30%, which may be ascribed to non-uniform concentration distribution due to the particular geometry of the reactor, thus contradicting one of the major assumptions of LH model. A tuning methodology based on an extensive CFD simulation procedure was applied to adjust the kinetic model parameters towards a better correspondence between simulated and experimentally obtained data. To validate the prediction accuracy, the kinetic simulations of heterogeneous photooxidation of NO_x were repeated with the optimized parameters, achieving a high degree of consistency (less than 3.4% of difference) with the experimentally obtained conversion.**

Keywords — CFD modelling; Photocatalytic Oxidation Process; User Defined Function; ANSYS/Fluent; Langmuir-Hinshelwood (LH) mechanism; NOx, heterogeneous surface reaction.

ACKNOWLEGEMENTS

The present study was developed in the scope of CICECO-Aveiro Institute of Materials, FCT Ref. UID/CTM/50011/2019 and Smart Green Homes Project [POCI-01-0247-FEDER-007678], a co-promotion between Bosch Termotecnologia S.A. and the University of Aveiro. It is financed by Portugal 2020 under the COMPETE Program, and by the European Regional Development Fund.

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The Rare Earth Oxysulfates And Their Energy Storage Potential

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***Abstract*— Battery stacks have always been one of the candidates to shoulder energy storage, especially electricity storage responsibility. Those huge battery stacks for electricity storage and conversion are sophisticated, expensive, and important. For example, NaS battery stack and Li-ion battery stack have been on the market over a decade[1]. Nonetheless, besides of the system sophistication, low unit power density and high price issues, the most important one is that NaS and Li-ion battery are not safe due to the use of reactive metal and liquid electrodes/electrolytes which hold the possibility of explosion1. We aim to develop an innovative electrochemical device for storing electrical energy generated through renewable sources, such as solar panel, wind farm, and oceanic tides, etc. This device offers the theoretical capacity of 1300mAh/g (5 MJ/kg), which operates at 500-900 °C[2]. The research deals with challenges of developing novel energy storage materials of rare earth oxysulfates that offer high energy capacity, stability, cyclability and safety.**

The battery design is as indicated in Fig.1. This device has potential to be used as grid-scale battery storage system if properly scaled up. It combines the solid oxide fuel cell and air-metal battery to form a hybrid stack. The device has to be run at elevated temperatures making it ideal to co-generate heat and electricity as well as increasing the round-trip efficiency. We finished the 1W battery power output in the lab and now move to 1000W trial. It is hoped the Rare Earth Oxysulfates battery stack can be a revolution for the renewable energy sector.

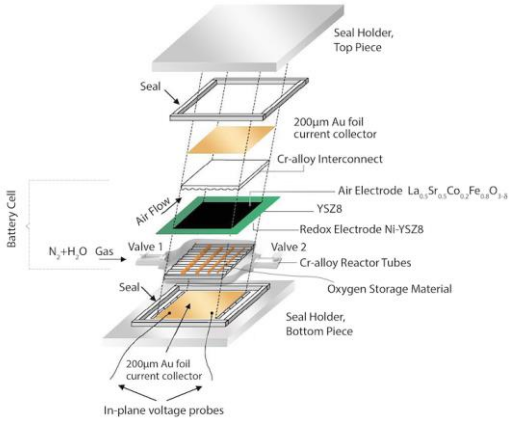

Figure1- Battery unit design.

Keywords - ceramic membrane, electricity storage, oxygen storage, recharging battery.

ACKNOWLEGEMENTS

This work is supported by the projects: UID/EMS/00481/2019-FCT - FCT - Fundação para a Ciencia e a Tecnologia; and CENTRO-01-0145-FEDER-022083 - Centro Portugal Regional Operational Program (Centro2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund.

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SUSTAINABLE MANUFACTURING SOLUTIONS

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Effect of ammonolysis temperature on physical properties of vanadium (oxy)nitride as a potential electrocatalyst for ammonia decomposition: synthesis, crystal structure and electrical properties

Laura Holz, Francisco J.A Loureiro, Vanessa C.D Graça, Sergey Mikhalev, Diogo Mendes, Adélio Mendes, Duncan P. Fagg

Abstract

Ammonia (NH_3) is considered as a potential energy carrier to be used as a fuel in energy conversion devices, such as solid oxide fuel cells (SOFCs). These eco-friendly systems can directly convert chemical energy into electricity. However, a key challenge still remains for finding alternative anode materials, aiming to improve the durability and the performance of the cell components. Hence, the present work is dedicated to the synthesis and characterization of vanadium oxynitride ($VO_{1-x}N_x$), as a potential novel rare earth-free anode material for NH_3-SOFC. The rock-salt structure ($Fm\bar{3}m$) of $VO_{1-x}N_x$ can be simply formed when V_2O_5 reacts with gaseous NH_3 in the temperature range 600 – 1000 °C. X-ray diffraction and Rietveld refinement reveal that the unit cell volume increases with increasing the ammonolysis temperature, being concomitant with the increasing amount of nitrogen incorporated into the anionic sublattice measured by thermogravimetry. The use of lower ammonolysis temperatures is, therefore, beneficial to obtain small crystallite sizes, with increased lattice strain, as measured by *Halder Wagner* method. The material exhibits a very high electrical conductivity in reducing conditions (1120 S·cm^{-1} at 800 °C), showing a slightly negative (E_a=0.04 eV) dependence with temperature, which evidences its typical metallic behavior.

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Description

Ammonia is considered a promising candidate as hydrogen carrier since it has high energy density, high hydrogen content, and no emission of CO_2 during decomposition[1]. For direct ammonia fuel cell, up to date, the best approach is to operate at high temperature using a SOFC (Fig.1) since the thermal decomposition of ammonia itself occurs at temperature above 550 °C[2]. The main challenge is the integration of redox stable anode in order to improve the durability of the anode/electrolyte interface and to achieve a good electrochemical performance[3]. In particular, transition metal oxynitrides, known as interstitial alloys, have been considered a fascinating class of materials due to their emerging applications as catalysts for ammonia decomposition and excellent electrical conductivity having similar properties to the platinum group metals[4].

1. General Description

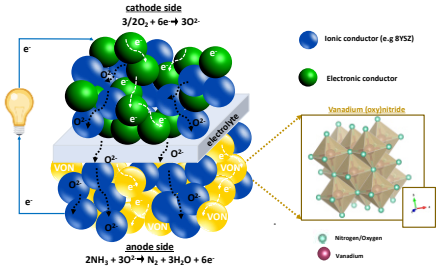

Fig 1 / Schematic representation of ammonia fueled SOFC. Rock-salt structure of vanadium (oxy)nitride material.

The rock-salt layered was confirmed by XRD refinement technique. The observed diffraction peaks (Fig. 2/ a.1) are indexed with a cubic structure, space group $Fm\bar{3}m$. The lattice parameters *a,b,c* gradually increase resulting in an expanded unit-cell as ammonolysis temperature increases, reflecting a peak shift towards lower diffraction angles on XRD patterns (Fig 2/a.2-a.3). Since the anionic radius of N^{-3} ion (146 pm) is larger than that of the O^{2-} ion (138 pm), the substitution of large sized N^{3-} ions to O^{2-} sites contributes to lattice expansion. The material exhibited an extremely high electrical conductivity (Fig.5) in reducing conditions (1120 S·cm^{-1} at 800 °C in 10 % H_2- 90 % N_2) when compared with selected anodes reported on literature (Table 1). Furthermore, it showed a slightly negative dependence with temperature which evidences the typical metallic behavior of this class of materials.

2. Structural characterization – XRD and Rietveld Refinement

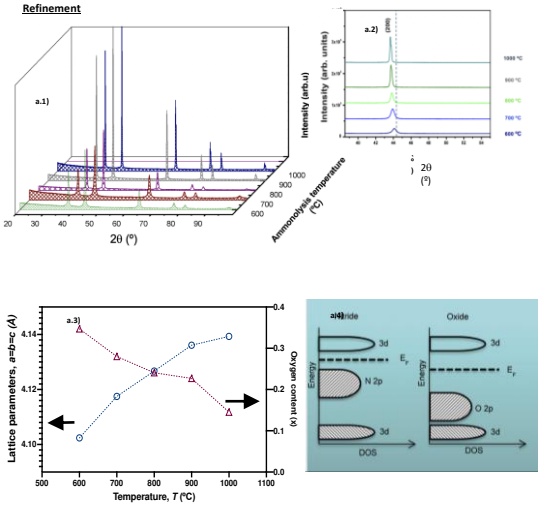

Fig 2 /a.1) XRD patterns of materials prepared at 600, 700, 800, 900 and 1000 °C. a.2) XRD patterns showing the peak shift. a.3) Lattice parameters and oxygen content determined as function of temperature. a.4) Schematic diagram of band energies for a semiconducting, late transition metal nitride and oxide (charge transfer type)[5].

3. Crystallite size and lattice strain – *Halder Wagner method*

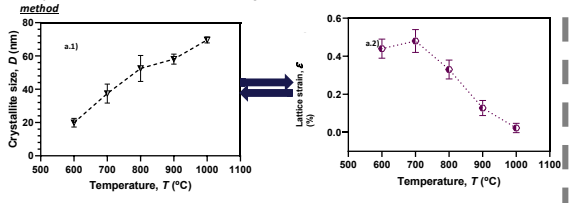

Fig 3 /a.1) Crystallite size and a.2) lattice strain as a function of ammonolysis temperature measured by Halder-Wagner method.

4.Powder morphology – SEM

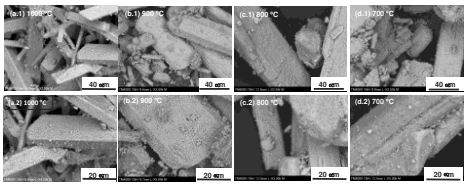

Fig 4 / SEM micrographs of $VO_{1-x}N_x$ powders synthetized by ammonolysis route at (a.1-a.2) 1000 °C (b.1-b.2) 900 °C (c.1-c.2) 800 °C (d.1-d.2) 700 °C.

5. Electrical properties in reducing conditions

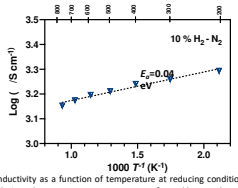

Fig 5 / Electrical conductivity as a function of temperature at reducing conditions (pO_2 < 10^{-21} atm) of VON sintered at 1200 °C during 5 hours. Measurements were performed by 4-probe DC method.

Table 1 / Electrical conductivity (σ) of selected conducting SOFC anodes at 800 °C measured in reducing atmosphere.

Anode materials	σ (S cm^{-1}) @ 10 % H_2-N_2 @ 800 °C	Ref
$La_{0.6}Sr_{0.4}TiO_3$	96	6
$Sr_{0.895}Y_{0.07}TiO_3$	7-64	7
$SrTi_{1-x}Nb_xO_3$	9-28	7
$Sr_{0.895}Y_{0.07}TiO_3$	7-64	6
VON	1120	This work

6. Concluding remarks

- Ammonolysis temperature is a key experimental parameter that determines the crystal structure, composition, crystallite size and lattice strain of vanadium oxynitrides;
- The use of lower synthesis temperature is beneficial to obtain lower crystallite size (20 nm) with higher lattice strain (0.4 %);
- Unit cell volume increases with increasing of nitrogen content on anionic sublattice;
- The material exhibited a very high electrical conductivity (1120 S·cm^{-1} at 800 °C) in reducing conditions (pO_2 < 10^{-21} atm), showing a slightly negative dependence with temperature which evidences the typical metallic behavior of this class of materials

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Exploring NbN material as electrocatalyst for ammonia synthesis by ammonolysis route

Vanessa C. D. Graça, Laura Holz, Sergey Mikhalev, Francisco J. A. Loureiro, Duncan P. Fagg

Abstract

Interest in ammonia (NH_3) synthesis research has been increasing over the past years due to its valuable application in many products. Ammonia is a chemical building block for the fabrication of plastics, explosives, pesticides, fertilizers, etc. Moreover, due to its very high energy density, it has also been considered as an alternative carbon-free fuel that can play a crucial role in a sustainable energy future.

The current industrial process for NH_3 synthesis is the *Haber-Bosch* process (HBP), however, this process is estimated to be responsible for 2.5 % of worldwide greenhouse-gas CO_2 emissions. To solve this problem, research has been focusing on alternative fabrication technologies, where one of the most promising is the electrochemical synthesis of ammonia.

However, one of the key limitations of the electrochemical ammonia synthesis is to find suitable catalysts for to break the nitrogen molecule. Transition metal nitrides ((TM)N) have been highlighted by DFT calculations to offer high catalytic activity for the ammonia formation reaction, whilst suppressing H_2 evolution (HER) [1], although experimental validation is currently lacking.

Hence, in this work, we aim to study the synthesis and stability of niobium nitride as potential electrocatalyst for ammonia synthesis using X-ray diffraction and thermogravimetry.

Description

Electrochemical ammonia synthesis uses the electrochemical cell illustrated in Fig. 1. Here, the cell is composed by an electrolyte proton-conducting membrane, sandwiched between two electrodes. The reactants (H_2 or H_2O) are dissasociated on the anode electrode, and the resulting protons diffuse across the membrane to the cathode electrode, where they react with gaseous N_2 to form ammonia.

The main interest of the current work is to develop alternative catalyst materials to be employed in the cathode. Hence, this component will be formed from a composite of a proton conducting phase and transition metal nitrides, Fig.1. This concept is based upon the knowledge provided from solid oxide fuel cells that has highlighted an increased electrochemical performance in mixed ionic and electronic conducting composite electrodes due to an extension of charge transfer reactions throughout the electrode bulk [2].

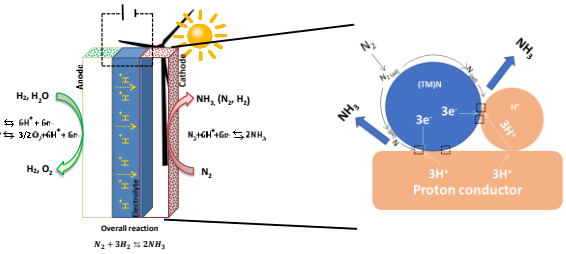

Fig. 1 - Working principle of electrochemical route for ammonia synthesis based on proton conducting solid electrolyte (right side) and a scheme of TPB regions for a mixed electronic ionic conductor proposed cathode (left side).

Methodology

There are many different processes for the formation of transition metal nitrides, with the most commonly used being the ammonolysis route. This procedure consists of a reductive nitriding treatment under a gas flow of NH_3 or a mixture of N_2:H_2 and the corresponding metal oxide precursor[3]. Fig. 2 shows the thermodynamic requirements for ammonolysis of some suggested transition metal nitrides. The Ellingham-Richardson-Jeffes diagram is useful for comparing the feasibility of the production of nitrides catalysts from a variety of oxides by ammonolysis as a function of temperature. Abghoui and colleagues[4] found that the most promising transition metal nitrides in terms of stability, activity and selectivity for the reduction of nitrogen to ammonia at room temperature and at ambient pressure are NbN, VN, CrN, RuN and ZrN.

Thermodynamic calculations

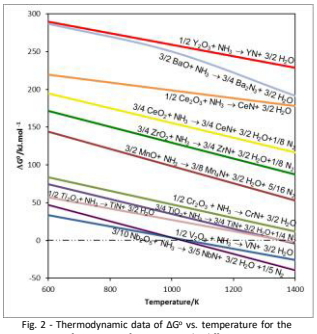

Fig. 2 - Thermodynamic data of ΔG^o vs. temperature for the reaction of ammonia formation with different transition metals oxide precursors. The thermodynamic requirements for ammonolysis of some suggested transition metal nitrides. All ammonolysis reactions show negative slopes indicating more favorable reaction with increasing temperature. The suggested transition metal nitrides are also indicated to be more likely to be formed by ammonolysis than BCZY, suggesting that the proton conducting phase will remain intact during this process.

Ammonolysis synthesis

Niobium nitride was successfully produced using this simple method, as shown by X-ray diffraction pattern in Fig. 3. In detail, the precursor of niobium oxide (Nb_2O_5) was directly converted to niobium nitride (NbN) using a dry NH_3 flow at 1000 °C for three hours in a tubular furnace. Before and after the thermal treatment, the tube furnace was purged with N_2.

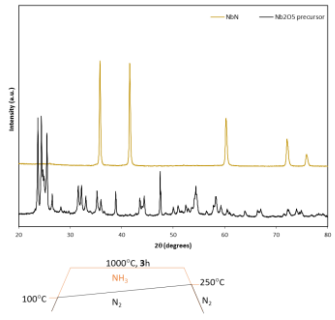

Fig.3 - X-ray diffraction patterns of the precursors (Nb_2O_5) and the NbN product obtained after ammonolysis.

Chemical stability of niobium nitride in N_2

To use transition metal nitrides as potential NH_3 formation electrodes, they should be stable in the working conditions. To test the stability of thermogravimetry in N_2 for 12h was performed. The results show that niobium nitride is not stable at 450 °C in N_2 while stability in 10%H_2/N is maintained. Therefore, binary and ternary system are currently under study to increase the material stability. [2]

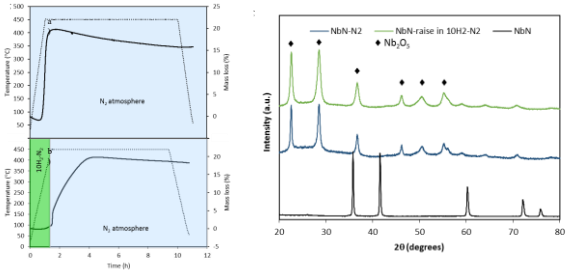

Fig. 4 – a) TGA profiles obtained from NbN in a) dry N_2 atmosphere and b) dry 10%H_2-N_2 atmosphere with change to pure N_2; b) X-ray diffraction patterns after performing TGA showing oxidation of NbN to Nb_2O_5.

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Acknowledgments

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TECHNOLOGIES FOR THE WELLBEING

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Connected and autonomous vehicles in mixed traffic flows: assessing energy and emissions potential benefits

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Abstract

Under a likely transitional stage of co-existence of connected and automated vehicles (CAVs) and conventional vehicles (CVs), this study explores the potential effects of CAVs to reduce greenhouse gases (GHG) and pollutant emissions in different road types based on improved operational parameters. Therefore, CAVs were assumed to behave like eco-driving agents to influence the environmental performance of overall traffic. A microscopic traffic and emission model platform was applied to simulate a European medium-sized city during the morning peak period. Four roadway sections (one motorway, one rural and two urban) were selected to evaluate in detail the impact of CAVs in different road types and over different CAVs penetration rates. Depending on the type of road, the impact may be beneficial in terms of carbon dioxide (CO_2) and nitrogen oxides (NO_x) reduction (up to 20%), but may also be negative in more congested roads. In particular, results show CAVs benefits are more relevant in motorway (up to 30%) and rural (up to 20%) sections. Regarding urban roads, the benefits can reach 7% in NO_x emissions in relation to the baseline scenario.

Description

CAVs technology is expected to improve fuel economy and reduce emissions per unit of distance, mostly due to more gradual acceleration/deceleration patterns and fewer stop-and-go movements.

Previous research in simulating vehicle automation has focused on understanding how driving behaviour parameters affect infrastructure capacity, energy consumption and emissions. Since CAVs technology is still under development, a widely used method in research is to adapt the current car following adjustment parameters (CFAP) and lane change models to simulate the impact of CAVs operation on the network.

Some studies assume that CAVs can incorporate car following adaptive algorithms to achieve secondary objectives such as minimizing emissions. Although, existing studies pointed out that significant reductions in emissions and fuel consumption can be obtained with the introduction of CAVs, little is known in how CAVs and CVs will co-exist and perform during a transitional stage.

Energy and Emissions Impacts of Connected and Autonomous Vehicles

- ✓ Reductions can be **expected** after CAVs replacing CVs;
- ✓ Research has been focused on **car-following** and **lane-change** behaviour parameters using simulation to minimize emissions/energy

Research Questions

Impacts of CAVs few explored in mixed traffic with CVs

i. **What are the potential reductions in CO_2 and NO_x emissions, resulting from CAVs operating in different road types?**

ii. **How can network-wide emissions and fuel consumptions vary according to different market penetration (MPR) of CAVs?**

iii. **Can CAVs influence energetic and environmental performance of CVs on different road types?**

Methodology

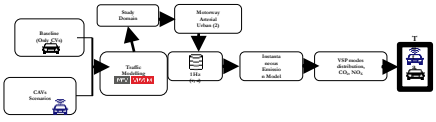

Fig. 1 Methodology overview

Model assumptions

Table 1 Summary of the assumptions made in this work

Demand	CAVs **do not affect** the matrix demand or vehicle occupancy rate
Street Design	CAVs operate in **mixed regime** with CVs (no dedicated lanes)
Emission Standards	CAVs have propulsion technology and emission standards **similar to** CVs
Driving Algorithms	The changes in vehicle movement result from technology/algorithms implementation **assuming optimal values** found in literature for CAVs.
Automation and Connectivity Level	V2V and V2I communications **not simulated**, but in some motorway segments CAVs **can adapt speed** to minimize emissions. CAVs are **levels 3 or 4** and can operate **without restrictions**.

This model assumptions are aligned with the research conducted by Greenwald & Kornhauser (2019) who anticipates that individually owned AVs would likely have the same per-vehicle-distance emissions as individually owned CVs.

Emissions Modelling

Emissions ⇨ Vehicle Specific Power (VSP)

Second-by-Second **Speed**, **Acceleration**, **Grade**

$$VSP = v \times \left[1.1 \times a + 9.81 \times \sin\left(\arctan\left(grade\right)\right) + 0.132\right] + 0.000302 \times v^3$$

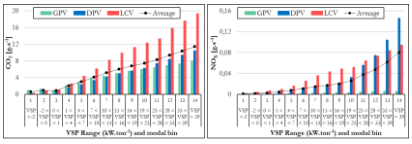

Fig. 3 Weighted average and emission factors used to estimate a representative vehicle of local fleet (Fernandes et al., 2018)

Case Study

- Aveiro, Centro Region, Portugal
- 14 traffic monitoring points (8.15-9.15 AM) and 550 km of vehicle dynamics (Bandeira *et al.*, 2018)

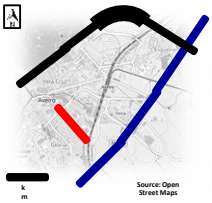

Figure 2 Aerial Map of Aveiro

Section C – Motorway

- 5.1 km in length
- 2 lanes by direction
- 120 km/h speed limit
- 1,560 – 3,250 vph

Section B – Arterial/Rural

- 4.5 km in length
- 1-2 lanes by direction
- 70 km/h speed limit
- 1,400 – 2,500 vph

Section A – Urban

- 0.6 km in length
- 1 lane by direction
- 40 km/h speed limit
- 900 – 1,300 vph

Car following adjustment parameters

Table 2 CFAP values used

CFAP	Reference	Arterial	Freeway 90 km/h	Section A Adjusted
CC0 [m]	1.50	1.47	0.5	(0.5;1.5;2.5)[2]
CC1 [s]	0.9	1	1	(0.5;0.9;1.5;2)[2]
CC2 [m]	4	0	0	0[1]
CC3 [s]	-8.00	-13.54	-4.00	(-4;-8;16)[2]
CC4 [m/s]	-0.35	-0.13	-0.10	-0,10[1,2]
CC5 [m/s]	0.35	0.13	0.10	0.10[1,2]
CC6	11.44			0[1]
CC7 [m/s^2]	0.25	0.08	0.45	0.05[1,2]
CC8 [m/s^2]	3.50	3.72	3.90	(3.1;3.5;3.9)[2]
CC9 [m/s^2]	1.50	1.60	1.90	--

An additional sensibility in CFAP values in section A was conducted to minimize NOx values during a 24-hour period. For that purpose, a Python-based code was developed in order to allow parameters that minimized NO_x emissions, for each different scenario.

Mobility Scenarios

BS – Only	
S1 – 90%	10%
S2 – 70%	30%
S3 – 50%	50%
S4 – 30%	70%
S5 – 10%	90%

[1] CoExist project
[2] Scenarios

Results

Average emission factors for different sections and scenarios

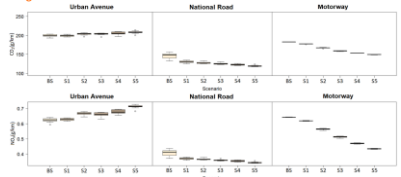

Figure 4 Average emission factors (g/km) per vehicle by scenario

Comparison of the total CO2 and NOX emissions of CAVs and CVs

Urban avenue:

- > 200g/km CO2;
- Significant reductions in emissions with an increase in the number of CAVs (between 3 and 18% for CO2, and 4 and 32% for NOx).

Motorway:

- Linear relationship between the share of CAVs and the effect on the reduction of CVs emissions (R2 = 90%).

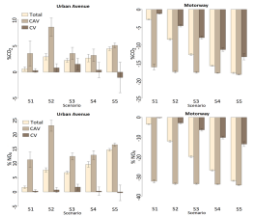

Fig. 5 Comparison of CO_2 and NOx by road and scenario

Scenarios comparison – NOx total emission

Fig. 6 Comparison of NO_x in 24-h period by scenario

- CC0 and CC1 did not show significant variations;
- CC3 and CC8 registered variations during the different periods within the 24-hour monitoring.

NOx emission reduction

Table 3 NOx emissions by scenario

CFAP	% NOx reduction (vs. previous scenario)	% NOx reduction (vs. baseline scenario)
S1	-2.10	-2.10
S2	-1.65	-3.71
S3	-1.70	-5.35
S4	-1.08	-6.37
S5	-0.92	-7.22

- S1 with most significant reduction of NOx (~2%).
- As suspected, NOx reduction is not so evident after S4.

Conclusions

i. What is the potential reduction of CO_2 and NO_x resulting from CAVs operating in different road types?

- ✓ Environment in the **arterial/rural section** (up to 12%);
- ✓ **Urban corridor**, the impacts revealed **positive**: 2% NOx reduction;
- ✓ Motorway segment, an optimization of the **speed to 90 km/h** => **- 18% of CO_2** and **- 32% NOx**.

ii. How can network-wide emissions and fuel consumptions vary according to different market penetration of CAVs?

- ✓ Outside the urban context, a relationship between emissions reduction versus MPR **was very good**. Most negative impacts for **30% of MPR**;

iii. Can CAVs influence the energetic and environmental performance of CVs on different road types?

- ✓ CAVs had significant influence on both energetic and environmental performance of CVs, ranging from 3 to 13%.

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NeuroStimSpinal

A Step Forward To Spinal Cord Injury Repair Using Innovative Stimulated Nanoengineered Scaffolds

Paula Alexandrina de Aguiar Pereira Marques

FUNDING

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Type of action: RIA

NEUROSTIMSPINAL COORDINATION

University of Aveiro

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NEUROSTIMSPINAL TEAM

The consortium comprises seven partners from four European countries: Portugal, Spain, the Netherlands and Greece and includes two industrial partners.

MEMBER	COUNTRY
University of Aveiro	Portugal
Tecnalia Research & Innovation	Spain
Universidade Complutense de Madrid	Spain
Radboud University & Radboudumc Stichting Katholieke Universiteit	Netherlands
Institute of Electronic Structure and Laser Foundation for Research and Technology – Hellas (Forth)	Greece
Graphenest – Advanced Technology (SME)	Portugal
STEMMATTERS – Biotecnologia e Medicina Regenerativa, SA	Portugal

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MOTIVATION

Spinal cord injury (SCI) has dramatic lifetime consequences affecting thousands of people worldwide. SCI results in para- and tetraplegia caused by the partial or complete disruption of descending motor and ascending sensory neurons. It leads to devastating effects such as sensory loss, paralysis and bowel/bladder dysfunctions. Different strategies have been proven at research level. However, today there is no effective SCI therapy that can entirely restore neuromotor deficit.

AIM

NeuroStimSpinal project aims at developing a treatment for patients after spinal cord injury (SCI) by at developing a neural tissue engineered scaffold capable of not only combining fibrous and porous topographic cues in order to mimic the morphology of the native spinal cord, but also potentiating the properties of graphene-related materials supported in a protein-rich decellularized matrix.

OBJECTIVES

- Formulation of different adECM/GBM compositions, shapes and porosity matrices rationally designed for different SCI locations
- Assess the biocompatibility, bio-functionality, performance (including electrical stimulation) of adECM/GBM scaffolds using embryonic neural progenitor cells (ENCPs)
- Evaluate the systemic and long-term efficacy of cell-laden and non-cell-laden scaffolds with and without electrical stimulation using rat and rabbit in vivo models

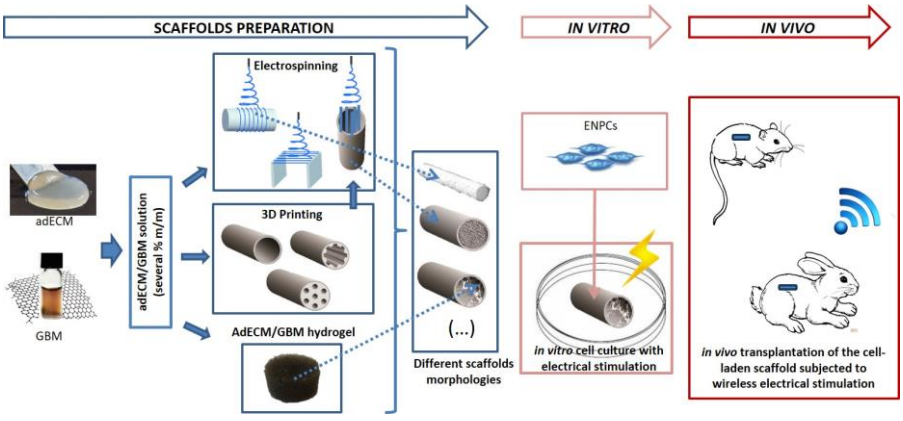

Figure 1. Schematic representation of the scaffolds design towards *in vitro* and *in vivo* experiments.

RATIONALE BEHIND SCAFFOLDS DESIGN

White matter tracts of the spinal cord form a highly organized tissue. Mature axons are highly aligned, and this architecture is essential for healthy cells behaviour and tissue function. After an injury, neurons processes grow in a disorganized manner, inhibiting an appropriate reconnection past the lesion cavity (see Figure 2).

Scaffolds for SCI must guide the injured axons with physical cues to grow (see Figure 3). Scaffolds will display aligned porosity to direct appropriate axon growth using various techniques such as electrospinning, 3D printing and freeze-drying.

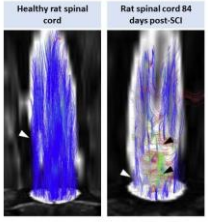

Figure 2. Healthy vs post-injured spinal cord in rats. Reference: Magnetic Resonance Imaging, 47 (2018) 25-32

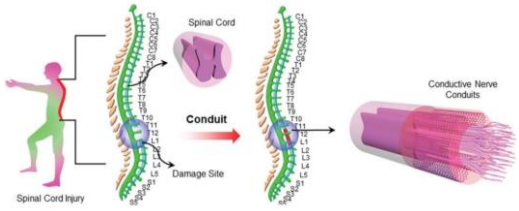

Figure 3. Schematic demonstration of the spinal cord in the human body and conductive nerve conduits for the treatment of injury. Reference: New J. Chem., 42 (2018) 17671

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