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PLENARY LECTURES

PAST, PRESENT AND FUTURE OF CFD

Akshai K. Runchal and Madhukar M. Rao
CFD Virtual Reality Institute, USA

Computational Fluid Dynamics appears to be poised on the threshold of rapid advances powered by the recent developments in Artificial Intelligence, Neural networks and deep machine learning. From the diversity of its use today, it is hard to believe that it originated just about 50 years ago. CFD is where it is today because of the contributions of two brilliant scientists. The science that led to CFD started at Los Alamos under the direction of Frank Harlow who was the first to realize the potential of emerging electronic computers to obtain solutions to the previously “unsolvable” problems governed by the Navier-Stokes equations. But it was the engineer in Brian Spalding at Imperial College who saw the potential of transforming this field engineering. Spalding worked with his team to unify the concepts of fluid flow, heat and mass transfer and developed general purpose software tools that have become the mainstay of modern engineering practice. This field of engineering software later became known as CFD. Majority of CFD simulations today employ the Finite Volume Methodology developed at the Imperial College, London, in the mid to late 1960’s and early 1970’s.

Early applications of CFD were largely in the field of aerospace and defense. However, in the last 5 decades, there is hardly a field of human endeavor that is untouched by CFD. It has become a pervasive and highly useful tool to understand the physics behind a diverse range of applications in engineering and science. This understanding, in turn, has led to innovations and improvements in a variety of fields. The applications of CFD have expanded to include areas such as biomedical, sport, food processing, environmental, fire safety, buildings ventilation and energy efficiency, and a host of other areas of social relevance. The uses of CFD today extend from understanding plate tectonics deep underground, to exploring exo-inhabitation in outer space and exoplanets. It is used to understand the diffusion of drugs deep in the human body and to designing novel systems to ameliorate the environmental and energy crisis facing human existence.

The limitations of the current generation of CFD tools fall in three broad categories. First, for many practical applications, the current CFD methodologies require computational resources that are beyond those available; hence compromises have to be made. Second, the current generation of tools are not robust; they require judgment from trained experts in CFD to ensure that the results are reliable. Finally, the current generation of CFD software lacks intuitive and easy to use human interface backed up by required auxiliary data that is needed to solve a problem. Therefore, extensive training is needed to use CFD tools effectively and accurately. This is expensive.

A number of new technologies have emerged and are entering mainstream that will transform the CFD tools of tomorrow. The foremost amongst these is deep machine learning. Deep machine learning (ML) is an artificial intelligence (AI) technology that is powered by recent advances in deep neural networks. A recent innovation is the physics-informed neural network (PINN) which incorporates the residual of governing equations as part of the cost function to be minimized while “training” the neural network. The PINN in conjunction with reduced order models, digital twins and internet-of-things (IOT) will have a profound impact on how products are designed, manufactured and serviced. It will be possible to embed ML into CAD/PLM software and even spreadsheets. This will enable engineers to rapidly assimilate these models into the product development process and thereby create optimal designs, without needing the services of a CFD expert. This technology will also be used for optimal control and real time monitoring of the device. All this will have a profound impact on the way that CFD is practiced and utilized. In short, CFD will become ubiquitous but at the same time deeply embedded within systems and devices, so a practicing engineer can use it without having to understand the nitty-gritty of CFD. CFD will become like the engine that drives a car but the driver rarely has to deal with it. CFD experts will be more engaged in creating the digital twins and reduced order models using high fidelity computations and of course, in extending the application of CFD into diverse areas of human activity.

Dr. Runchal has seen the CFD emerge in the 1960’s as an esoteric and niche research field that evolved into its vibrant and multi-disciplinary state today. He was part of a group of 3 students who worked with Prof. Spalding at Imperial College to develop the FVM methodology. He has been a practicing CFD engineer since then. Dr. Rao has been a developer of CFD algorithms and technology and has been a practicing engineer for over 35 years. This talk is based on their experiences in this field and their thoughts on how it is evolving.

ADVANCES IN EXPERIMENTAL AND COMPUTATIONAL ANALYSIS OF THE NEONATE'S BRAIN COOLING PROCESS

Andrzej Nowak
Silesian University of Technology, Poland

According to the World Health Organization, perinatal asphyxia (PA) represents the 3rd most common cause of neonatal death. This means that all over the world, almost 600,000 newborns die every year, and at least as many develop hypoxic-ischemic encephalopathy (HIE), which is one of the most common causes of severe neurological deficits in children, presently in approx. 15 out of 10,000 live births.

Among the various methods tested for efficacy in newborns with PA, therapeutic hypothermia (TH) has proved to be useful in clinical practice and to be effective in protecting the brain against the effects of ischemia/hypoxia. Generally, there are two main types of TH: selective TH carried out using cooling cap and whole body TH in which cooling pad (or blanket) is used. They are schematically demonstrated in Fig.1.



Fig.1. The selective and whole body Therapeutic Hypothermia

Although, each specific TH has its own peculiarities, there are several actions/steps which are very similar and important from a heat transfer point of view. In both cases, the newborn is placed in an open incubator, and in both cases, the treatment lasts 72 hours. The essence of TH is to maintain the newborn's core temperature at a reduced level, which in the case of selective head hypothermia is 34-35°C, and 33-34°C in the case of whole body hypothermia. This can be achieved in different ways, depending on the type of cooling device.

In this presentation the heat transfer processes occurring during both, the selective TH as well as the whole body TH will be described and compared. The non-invasive thermal measurements of temperatures and heat fluxes occurring during cooling therapy will be presented and discussed. They will also be subject of the cumulative energy balance which seems to be a new method of assessing the thermogenesis of infants with HIE undergoing TH. Calculated in this way the metabolic heat flux can be used to improve the process of therapeutic hypothermia. Finally, based on those cumulative energy balances, so-called Thermal Index become a candidate for an indicator (predictor) that can help in the assessment of the degree of brain injury and in the prognosis of the patient's condition after treatment.

ACKNOWLEDGMENT

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PORE SCALE ANALYSIS OF THERMAL AND FLUID DYNAMICS BEHAVIORS IN OPEN METAL FOAMS

Bernardo Buonomo, Anna di Pasqua, Oronzio Manca, Sergio Nappo, Sergio Nardini, Safa Sabet
Università degli Studi della Campania "Luigi Vanvitelli", Italy

The investigation of fluid flow in porous media has been of great interest for engineers and scientists in recent years. Many applications, such as in refrigeration, automotive, aerospace, process industry and heat exchangers, energy systems and thermal energy storage use porous media to increase thermal performance. Metal foams are a new type of material and are used to improve heat exchange in many components and systems. The related behavior is influenced by the structure of the foam and by parameters such as diameters of cells, struts, and pore density, the shape of struts and the porosity. The structure can be realized by a forming technological process or by additive manufacturing (AM) it is non-ordered-random (stochastic) structure or AM-ordered structure, respectively. The structures present different fluid dynamic and thermal characteristics. The huge applications in heat transfer of metal foams, both stochastic and AM-ordered, and the need to improve the convective heat transfer performances are determining to understand better the phenomenology more in depth to evaluate the pressure drop and local heat transfer coefficient at pore-scale level as underlined in literature. In the present investigation an analysis on Kelvin cells which can represent both the stochastic foam and the ordered foam is accomplished to analyze different characteristics with phase change materials, low pressure gas cases or microscale systems, and nanofluids. Some results related to the entropy generation analysis are also presented.

MODELING OF LIQUID METAL FLOWS DURING ASSEMBLY OPERATIONS AND CHARACTERIZATION OF THE PROPERTIES OF THESE METALS AT HIGH TEMPERATURES

Philippe Le Masson
Université Bretagne Sud, France

The assemblies of metallic materials can be made by welding, additive manufacturing or even sintering. Understanding operations covers several points. First, the input of heat and molten matter generates energy distribution and the flow of molten matter. Then, the metallurgical transformations (allotropic transformations, fusion, solidification...) lead to modifications of the intrinsic properties of materials (thermal, electrical, mechanical...). In addition, the molten material due to its composition and its gaseous environment sees its flow properties modified (surface tension, viscosity for example). Finally, the thermal evolution jointly with the metallurgical transformations induce mechanical consequences in terms of residual stresses and strains.

The simulation of assembly operations will therefore be built by integrating either in a multiphysical form phenomena of energy input (arc, laser, etc.) and material (fusion of powder, wire, etc.), or in a simplified form to couple thermal, metallurgical and mechanical phenomena. Simulation examples will be presented.

Emphasis will be placed on the choice of parameters at high temperatures, emphasizing their effect on the results. The lack of data in the literature has led us to propose experimental developments in order to characterize metallic materials in the molten state. Examples of property measurements will then be presented.

COMPUTATIONAL METHODS OF DESIGN AND IDENTIFICATION OF THERMAL PROTECTION OF SPACECRAFT

Aleksey Nenarokomov
Moscow Aviation Institute, Russia

Methods of Inverse Heat Transfer Problems (IHTP) were developed to increase the amount of information from thermal experiments and tests, to improve the accuracy and reliability of experimental data processing and interpretation, and also for investigating and control of Heat Transfer in production processes. In the majority of cases this methodology is used for optimization but in a number of practical situations it is the sole technique available, as, for example, in measuring the transient heat fluxes and heat transfer coefficients. This methodology is based on the mathematical theory of ill-posed problems of mathematical physics.

One of the most important directions of studies where the application of methods of inverse problems is necessary is the design of thermal protection and identification of the heat transfer processes of spacecrafts. Under development is a new approach to the thermal design of high temperature thermal protection, based on the identification of nonlinear systems with distributed parameters. Proceeding from this approach modern experimental-computational methods have been developed to determine thermal, thermokinetic, radiative and other properties of various materials of complex composition, as well as corresponded methods of design.

Depending on the type and mission of the material the considered mathematical models of heat transfer can be divided into four groups:

1. Models of solid opaque materials with effective thermal characteristics depending on temperature and time;
2. Models with a high porosity of the materials or semitransparent fibers, etc.;
3. Models including the kinetics of destruction of composite materials and related processes;
4. Models of multilayer thermal insulation with applications to orbital spacecrafts.

COST-EFFECTIVE APPROACHES TO PREDICTIONS OF THERMOFLUID PHENOMENA IN ENGINEERING SYSTEMS

Bantwal R. (Rabi) Baliga, James I. Medvescek, Osaid Matar, Iurii Likhmanets, Laurent Mydlarski
McGill University, Canada

Cost-effective approaches to numerical predictions of thermofluid phenomena in engineering systems facilitate the elucidation of the underlying physics of these phenomena and the optimal designs of such systems. The term 'cost-effective' is used here to categorize approaches that allow predictions of acceptable accuracy and computational times (these are relative terms that require a suitable context for meaningful interpretation, as is elaborated in this presentation). The focus in this presentation is on hybrid approaches with the following key features: multi-dimensional mathematical models are used only in portions of the system where it is critically important to do so; in relatively simpler portions of the system, semi-analytical quasi-one-dimensional or quasi-two-dimensional models are used; and the numerical solutions of these models are iteratively coupled. In unsteady problems, such approaches could involve a combination of fully time-dependent and steady (or quasi-steady) formulations, when justified. Hybrid approaches involving combinations of analytical and numerical methods are not discussed in this presentation (instead, references are made to some related seminal and important contributions of several Brazilian researchers). Cost-effective hybrid approaches to numerical predictions of thermofluid phenomena have appeared in the published literature for over 25 years. In this presentation, excerpts from some recent works on such approaches to predictions of thermofluid phenomena in micro-grooved vapor-chamber heat spreaders, latent-heat (solid-liquid) thermal energy storage in plate-fin enclosures, closed-loop thermosyphons, interrupted-plate ducts, and thermal energy storage in rock beds are discussed.

INVERSE METHODS IN HEAT TRANSFER THROUGH MODELLING AND MACHINE LEARNING

Perumal Nithiarasu
Swansea University, UK

The re-emergence of machine learning methods creates many opportunities for the heat transfer community to transform understanding of heat transfer topics and heat transfer equipment design. The data-rich area the heat transfer researchers have created in the last fifty years enhances the opportunity to provide a new way of assembling information. More use of the connected world will reduce the need for duplicating or repeating experiments unnecessarily. This lecture will discuss a framework to use data more effectively in an inverse setting.

While the heat transfer community has been working hard on inverse problems, many issues such as multiple solutions and convergence are not fully resolved. These issues can be turned around into advantage when using machine learning. For example, multiple solutions can be an advantage in providing multiple choices of design. Thus, exploring machine learning options to carry out inverse modelling in heat transfer is important.

The first part of the talk will use simple examples of heat transfer and other problems to demonstrate how one can use machine learning in inverse modelling. Besides, how we can fill the data gap using a computational model will also be discussed. The talk will end with how the compact heat exchangers' data-rich area can benefit enormously from the available data if it can be gathered together. For example, the work will also demonstrate a forward deep learning method for offset strip fin heat exchangers.

DIRECT NUMERICAL SIMULATIONS OF HEAT TRANSFER FROM A CYLINDER IMMERSSED IN THE PRODUCTION AND DECAY REGIONS OF GRID TURBULENCE

George Papadakis
Imperial College London, UK

We consider a cylinder immersed in the turbulent wake of a grid-element and explore the effect of cylinder location on heat transfer using direct numerical simulations (DNS). Three locations downstream of the grid-element, inside the production, peak and decay regions, are investigated. The turbulence intensities at the location of the cylinder in the production and decay regions are almost equal at 11%, while in the peak location the turbulence intensity is 15%. Although the oncoming turbulent intensities are similar in the two regions, we notice a peculiar behaviour: in the production region the stagnation point heat transfer is increased by 63%, while in the decay region it is enhanced by only 28% (compared to the baseline case of approaching flow without turbulent fluctuations). Also, existing correlations for the stagnation point heat transfer coefficient are found to be invalid in the production and peak locations, while they are satisfied in the decay region.

In order to explain these findings, we study the flow structures and find that in the production and peak regions the flow is dominated by shedding events, in which the predominant vorticity component is in the azimuthal direction. This leads to increased heat transfer from the cylinder, even before vorticity is stretched by the accelerating boundary layer. Also, the frequency of oncoming turbulence in the production and peak locations lies close to the range of frequencies that can penetrate inside the boundary layer developing on the cylinder, and therefore the latter is very responsive to the impinging disturbances. The highest Nusselt number along the circumference of the cylinder is shifted 45 degrees from the front stagnation point. This shift is due to the turbulence-generating grid-element bars that result in the prevalence of intense events at the point of maximum Nusselt number compared to the stagnation point.

MINIMIZATION PROCEDURES FOR THERMAL PARAMETERS IDENTIFICATION FROM THE EXPERIMENT TO THE PHYSICAL MODEL

Jean-Luc Battaglia
Université Bordeaux, France

The thermal conductivity measurement of materials as thin films or nanostructured devices is still a challenging task. It is generally required to make the experiment suitable with the system to be characterized, avoiding thus the use of commercial apparatus that can only deal with “classical” configurations. In addition, the characterization of the thermal properties has to be performed within a large temperature range in order to highlight the most significant features of the materials with regards to its final application. We will illustrate our talk by considering phase change chalcogenide alloys, as GeTe or GeSbTe, that are used nowadays as the core material of non-volatile memories devices. Those alloys present a phase change between amorphous and crystalline state at a specific glass temperature. The huge electrical resistivity change observed between those two states is used to store a bit.

As a first step, we will illustrate how the inverse methods can be implemented in order to identify the thermal properties of such materials. Different contact and contactless experimental techniques have been developed in order to deal with such materials and devices. We will present the experimental methods we have used in our team: the modulated photothermal radiometry, the periodic pulse photothermal radiometry, the time domain thermoreflectance, the 3-omega and the scanning thermal microscopy. A model of the heat transfer within each experimental configuration has been developed and an inverse procedure has been implemented in order to identify the thermal parameters of interest. In this talk we will focus mainly on thermal conductivity and thermal resistance at interfaces.

Several models can be used in order to explain the identified thermal properties, ranging from first principal methods (ab- initio, DFT), molecular dynamics and models based on the phonon density of states using the expression of the phonon scattering relaxation time associated to each type of scattering (phonon-phonon, phonon-defects, phonon-electron, ballistic regime, ...). This later approach has led to the so-called Callaway, Callaway-Holland, Slack or Klemens models for instance. Those models are still widely used since they provide fast and reliable analysis of the thermal conductivity in a large range of temperature from 1K to the melting temperature. In this keynote, we will present the identification approach of the parameters involves within the relaxation time functions based on a complete sensitivity analysis and different minimization techniques.

LATTICE BOLTZMANN METHOD FOR MULTI-PHASE FLOWS

A.A. Mohamad¹, S.S. Baakeem¹ and S.A. Bawazeer²

¹The University of Calgary, Canada - ²Umm Al-Qura University, Saudi Arabia

One of the main advantages of the lattice Boltzmann method (LBM) over the conventional computational fluid dynamics (CFD) is its kinetic nature in dealing with the interface between the phases of fluid flow, which does not need to track the interface. There are four models to simulate multi-phase flows in the LBM: color-gradient, free energy, interface tracking, and Shan–Chen (SC). The color-gradient model has two distribution functions and an extra collision and re-coloring step. Also, it is suitable to specify the wetting conditions. One distribution function is used in the free energy model. However, the Poisson equation needs to solve for each time step. The interface tracking model has two distribution functions. Moreover, the free energy and interface tracking models are inconvenient to specify the wetting conditions. Owing to its simplicity and flexibility, the SC model is the most widely used in the open literature. The SC model has one distribution function and is convenient to specify the wetting conditions. Several approaches have been suggested to modify and improve the SC model, such as using higher-order isotropy, extending the single-relaxation-time LBM to multiple-relaxation-time LBM, coupling the SC model with the Equation of State (EoS), and enhancing the force term. The current work focuses on the SC model and its improvements.

NONLINEAR COMPUTATION: FUTURE OF NUMERICAL SIMULATION

Liqiu Wang

The University of Hong Kong, Hong Kong

Attempt to understand the world counts on our understanding of topics like bifurcation and chaos, and features like multiplicity, stability, and sensitivity with methods such as continuation and branch switching. “Nonlinear Computation” is a short name for “computation of something that is nonlinear”. It provides a framework for the computational science and engineering of the future and is essential when we try to predict and simulate the dynamics of states in the technical systems we utilize, in the ecological and economical systems we live, and in the biological systems we belong. In this lecture, I will discuss key issues in nonlinear computation and show its capabilities by using examples like (1) convection in microchannels, (2) cooling systems of rotating machinery, (3) microfluidic fabrication of smart materials, (4) thermal control system for the Alpha Magnetic Spectrometer (AMS) on the International Space Station, and (5) causative factors and the clinical applicability of spontaneous regression of malignant tumors.

GROWTH AND DYNAMICS OF VAPOR BUBBLES IN VARIOUS REGIMES OF BOILING WITH AND WITHOUT EXTERNAL ELECTRIC FIELD

Gautam Biswas

Indian Institute of Technology Kanpur, India

In the present investigation, we performed coupled level set volume of fluid (CLSVOF) based direct numerical simulations to predict the liquid-vapor instability, bubble generation, bubble growth and its departure during pool boiling. As a part of the process of bubble growth, the dynamical disturbances destabilize the liquid-vapor interface. The wavy interface culminates into vapor bubbles, which grow and finally buoy away. The instability mode transforms from Rayleigh-Taylor at the low wall-superheat temperature to Taylor-Helmholtz at the higher superheat values, altering the separation distances between the sites of bubble generation.

The discrete bubbles are observed at the lower range of superheat values while continuous vapor columns emanate in the cases of high superheat values. The detachment of the bubbles and the ebullition cycles follow a regular periodic pattern (in space and time).

Application of external electric field results in destabilizing the interface entailing the enhancement of the bubble growth rate. It is observed that the application of the electric field, normal to the heating surface, results in increase of both spatial and temporal frequency of bubble-formation along the heated surface. The dominant wavelength of disturbance decreases which in its turn decreases the separation-distance between the adjacent bubbles.

Thermal buoyancy is one of the pertinent parameters influencing the growth-dynamics of the vapor bubbles. The changes in the gravity-level result in a significant variation in boiling characteristics. Analyses have been performed at different levels of gravity to understand the changes in bubble morphology and heat-transfer rate.

The application of an external electric field compensates for the reduction in the heat transfer rate brought about by the condition of reduced gravity. During the initial stage of bubble growth, the interfaces exhibit self-similar profiles, i.e. the bubble interface at different instants of time can be converged on a single profile defined by a fitting function in which the variables are normalized using proper scaling parameters.

In the case of nucleate boiling, the bubble generation is not an interface-instability driven phenomenon but a random process which depends on the heat flux from the surface and the surface-properties. In this study, the growth rate is found to be affected by the surface-superheat, the wettability of the surface and the degree of subcooling of the ambient liquid.

MUTUAL INTERACTIONS OF EVAPORATIVE HEAT TRANSFER PHENOMENA AND WETTING PHENOMENA: NUMERICAL SIMULATION AND EXPERIMENTAL VALIDATION

Peter Stephan

Technische Universität Darmstadt, Germany

In many two-phase heat transfer processes, such as nucleate boiling, spray or drop impingement cooling, a superheated wall is in contact with a dynamically moving interface between the liquid and vapor phases of the heat transfer fluid. The local phenomena next to this moving contact line during the wetting or dewetting process strongly interact with the flow and heat transfer in the thermal boundary layer and vice versa. However, these mutual interactions are still poorly understood. How does the wall superheat or evaporation rate influence wetting/dewetting dynamics? And how do wetting/dewetting dynamics influence the evaporation rate? The plenary talk will address these interactions. A multiscale model was developed that combines the description of flow and heat transfer in the thermal boundary layer as well as in the bulk fluid with a subgrid model that describes the details of the non-isothermal wetting/dewetting phenomena. The model was implemented into the CFD platform interFOAM and applied to study single drop impingement cooling events as well as single bubble nucleate boiling events with high temporal and spatial resolution. Generic experimental setups were developed and used in parallel to validate the model and to compare experimental and numerical results. The model, the numerical procedure and the experimental methods are described. Comprehensive results are presented for the drop impingement cooling case. Numerical and experimental results agree well with each other. The extremely high resolution of the numerical results gives deep insights into the local phenomena near the wetting/dewetting front as well as the interaction with the bulk flow evolution and the heat transferred by transient conduction and evaporation.

SPECIAL SESSION IN
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CHT-21-BS-101 Development and applications of a high-order meshless method for fluid flow and heat transfer in complex domains, by **Surya P. Vanka**, S. Shahane, A. Radhakrishnan, M. Xu, P. Kumar, N. Bartwal, A. Unnikrishnan, S. Roy and V. Narayanan

In this talk, we will present development and applications of a high-order meshless method based on scattered data interpolation techniques. A complex domain is first represented by discrete scattered points generated by any method of choice. The flow variables are located at the scattered points, and interpolated over a local cloud of points using a radial basis function (RBF). Of the various RBF, we consider polyharmonic splines (PHS) which have the advantage of not needing a shape parameter as required by multiquadric (MQ), inverse multiquadric (IMQ) and Gaussians. We further append a polynomial of desired degree to achieve high order discretization accuracy. To solve the Navier-Stokes equations, the partial-derivatives are evaluated by differentiating the radial basis functions along with the polynomials. We have developed an explicit fractional step method and a semi-implicit method to integrate the Navier-Stokes and energy equations in time with high spatial and second-order temporal accuracies. The explicit fractional step method is limited by the combined convective and diffusive Courant number while the semi-implicit method can use time steps 10-20 times the explicit time step. In addition, we have developed a non-nested multilevel algorithm to solve the elliptic Poisson equation and applied it to solve heat conduction and pressure-Poisson equation in several complex geometries. In a collaborative effort between researchers at UIUC, Corning, IIT-Kharagpur, India and IIT-Gandhinagar, India, we have applied the three algorithms to several fluid flow and heat transfer problems in complex domains. We have demonstrated that the method has high spatial discretization accuracy.

CHT-21-BS-102 Computational-analytical integral transforms in transport phenomena, by **Renato Machado Cotta**

The Generalized Integral Transform Technique (GITT) is a well-established computational-analytical approach for linear and nonlinear diffusive and convective-diffusive partial differential formulations, which was mostly advanced in the realm of problems in transport phenomena. This presentation is a tribute to Prof. D.B. Spalding, who stimulated this research direction in private communications with the author, back in 1994, just after publication of his first book on this hybrid method in 1993. First, formal GITT solutions for nonlinear formulations are reviewed, including the alternatives of adopting nonlinear, coupled and/or convective non-classical eigenvalue problems, either on total or partial transformation schemes. Next, the GITT is formalized in the solution of the eigenvalue problem itself, including the direct integral transformation of problems defined in irregular domains, based on simpler auxiliary eigenvalue problems written for the same geometry. Then, a single domain reformulation strategy is discussed, which accounts for physical heterogeneities of the domain, by rewriting the different media transitions as space variable equation coefficients and source terms. These strategies are briefly illustrated through representative applications, exploring the convergence characteristics of the proposed eigenfunction expansions, towards the establishment of sets of benchmark reference results. This hybrid approach is also considered as an alternative general simulation tool, coined as the UNIT (Unified Integral Transforms) algorithm, and critically compared against results from purely numerical general purpose CFD codes.

CHT-21-BS-103 Direct numerical simulation of evaporating falling films in laminar gas streams, *by Avijit Karmakar and Sumanta Acharya*

Direct numerical simulations are performed to investigate the interfacial heat and mass transfer from evaporating falling films in laminar gas streams comprising of vapor and air. The full set of coupled liquid-gas flow equations (Navier-Stokes equations) are solved using finite-volume based approaches pioneered by Spalding and Patankar (1972) while the gas-liquid interface is resolved using the Volume-of-Fluid approach (Hirt and Nichols, 1981). The configuration considered is that of a falling liquid (water) film on a heated vertical plate with evaporation at the gas-liquid interface based on the gradient of vapor mass fraction. Two ambient conditions are considered: (a) co-current flow and (b) counter-current flow of gas. Interface instabilities are triggered using a small monochromatic forcing disturbance that leads to sinusoidal and solitary waves at the liquid-gas interface under respective forcing frequencies. The values chosen for the water inlet mass flow rate, water inlet temperature, the ratio of water to gas mass flow rate, and gas stream inlet temperature correspond to the available experimental data. The numerical predictions are seen to be in good agreement with the reported measurements. The resolved simulations examine the influence of interfacial waves and flow patterns on local Sherwood numbers and present the heat and mass transfer mechanisms taking effect in specific wave regimes.

CHT-21-BS-104 Recent developments in modelling of polymer electrolyte cells, *by Steven Beale, Shidong Zhang, Steffen Hess, Uwe Reimer, Norbert Weber, Holger Marschall and Werner Lehnert*

Polymer electrolyte electrochemical cells (PECs) offer exciting possibilities as energy converters in the form of both fuel cells and electrolyzers. Computational fluid dynamics can be used to analyse the performance of virtual prototypes at the micro-scale, as well as the cell and stack levels. This presentation details a comprehensive program of development of open source tools to describe and predict PEC operation. The software employed is OpenFOAM, which mimics the governing partial differential equations that describe the physics of PEC behaviour. Models range from detailed two-phase flow in porous transport layers based on digital reconstructions and the volume of fluid method, through single and multi-fluid cell models employing Eulerian-Eulerian solvers, to stack-level models whereby volume averaging also known as local homogenization is employed for both single-phase and two-phase formulations. The development of a multi-phase stack model represents an original and novel scheme not previously published. The results of mathematical calculations are compared with analytical solutions for one-dimensional idealizations, previous three-dimensional (3-D) numerical work by other researchers, and detailed experimental data gathered in-house. Comparisons are made in terms of local current density and species mass/molar fractions, as well as current density vs. voltage, i.e., polarization characteristics. Different levels of model complexity are also considered, for instance comparisons of a 2-D electrochemical formulation based on a Kirchhoff-Ohm equation (ideal potential less losses/over-potentials) vs. a fully 3-D simulation of both ionic and protonic potential fields. The presentation concludes with an assessment of the needs/requirements of the next generation of PEC analysis tools.

CHT-21-BS-105 Examples of computational fluid dynamics models for nuclear industry applications, by ***Milorad Dzodzo***

Validation of Computational Fluid Dynamics (CFD) models for industrial applications is more challenging due to the complex geometry and long duration and complexity of various postulated accident scenarios, resulting in different and wide ranges of length and time scales. Thus, CFD models for industrial applications are restricted to the smaller subdomains and short periods of postulated accident scenarios. Validation is most often based on the comparisons with experimental results obtained with the scaled down test facilities. Thus, the effect of scaling needs to be considered and incorporated in the validation process. During validation, valuable experience is gained related to geometry simplifications, needed mesh size, turbulence and heat transfer modeling, effects of initial and boundary conditions, different fluid thermophysical properties and interaction with other phenomena and processes. Based on the gained experience the validated CFD models are adjusted and used to simulate prototypical domains and conditions. Several examples of validations of CFD models for industrial applications are presented.

GENERAL **PRESENTATIONS**

CHT-21-101 A study of the melting of n-octadecane in horizontal cylindrical annuli: onset of convection and global melting, by **Mohammad Azad and Dominic Groulx**

In the present study, the melting of n-octadecane (a PCM with a melting temperature of 300.65 K) in horizontal cylindrical annuli heated at constant temperatures from the centre-tube was investigated numerically. The outer circumference of the annuli was insulated. COMSOL Multiphysics 5.3 was used to conduct the simulations using the modified heat capacity-porosity method, where the impact of the mushy zone constant was also evaluated. The diameters of the centre-tubes were 18, 27, and 36 mm; the initial temperatures of the PCM were 2.5, 7.5, 15 and 22.5 K below its melting temperature, and the temperatures of the heat transfer fluid (HTF), flowing through the centre-tube, were 8.4, 25.3 and 42.2 K above the melting temperature of the PCM. The Stefan numbers based on the differences between the temperature of the HTF and the melting temperature of the PCM were 0.1, 0.3, and 0.5. Correlations were developed for the onset of natural convection and for global melting. These results, as well as solid-liquid interfaces, were validated against in-house experimental results. The correlations for the onset of natural convection, derived from the numerical studies, are in-line with those obtained experimentally. In addition, the relationships of global melt volume with the different geometric and operational parameters derived numerically agrees well with the ones obtained experimentally.

CHT-21-102 Flow and heat transfer inside a rotating annular space, by **Ahmed M. Teamah and Mohamed S. Hamed**

Multiphase flow and heat transfer within a rotating annular space filled with air and oil has been investigated. Transient numerical simulations have been carried out using ANSYS-CFX. Numerical results have been validated using analytical results. The effect of rotational speed and oil volume fraction on the rate of heat transfer has been investigated. Rotational speed has a significant effect on heat transfer within the annular space. An optimum oil volume fraction has been identified.

CHT-21-103 An improved solution for shielding of thermal radiation of fires using mist curtains of pure water or sea water, by **Leonid A. Dombrovsky and Siaka Dembele**

An improved theoretical model for the shielding of radiation from large-scale fires by the mists of pure water or sea water is presented. This is a continuation of a recent study by accounting for both the partial re-absorption of infrared radiation in the absorption bands of gases and the variation of the incident radiative flux along the flame. As before, the solution to a combined problem of heat transfer consists of the spectral radiative transfer in a mist curtain, the kinetics of droplet evaporation, and convective heat transfer along the curtain. The previously suggested spectral models for optical properties of water droplets and salt particles formed by evaporation of sea water droplets are used in the calculations. The radiative transfer model is based on a set of not time-consuming 1-D numerical solutions across the mist curtain. The latter makes possible to perform a series of new calculations for both the uniform and two-layered mist curtains (with a distance between the curtain layers). Unlike in

our previous study, the radiative heat losses to the nozzle head and the floor under the curtain and the decrease in the downward velocity near the floor are accounted for the first time using the 2-D calculations. It is shown that radiative losses towards the floor and nozzle head are insignificant even for thick water curtains. Some recommendations on correct choice of parameters of two-layered mist curtains with relatively low total flow rate of supplied water are given. In particular, it is confirmed that the use of smaller droplets of water in the second layer of mist curtains reduces the total flow rate of supplied water at approximately the same attenuation of the flame radiation by the curtain. In terms of radiation shielding, it is also shown that the protection offered by sea-water curtain is almost the same as that of pure water. However, the use of sea water is potentially preferable for better protection from the fire radiation in the lower part of the curtain. The latter statement is correct in the case of high protective mist curtains, when the droplets of pure water evaporate completely before reaching the floor, whereas the hollow particles of sea salt are there in the lower part of the sea-water mist curtain. The study confirms that sea-water curtains can be used in coastal areas, offshore platforms or maritime transportation ships for shielding fire thermal radiation.

CHT-21-105 Transient response of different refrigerants used in single-pass dual chiller, by **Sambhaji T. Kadam**, Anaya Bara, Ibrahim Hassan, Mohammad Azizur Rahman, Athanasios I. Papadopoulos and Panos Seferlis

A number of process parameters can affect the performance of the district cooling plant, in which the vapor compression refrigeration (VCR) cycle has been widely employed. Two major process disturbances are: the end-user daily varying cooling demand (temperature of the received chilled water) and the seasonal changes in environmental conditions (cooling water temperature). This paper aims to investigate the effect of the selected refrigerants (R134a, R32, R717, R1234yf, R410a) on the transient response of dual chillers. It considers the cooling water temperatures as the process disturbances and disturbance are introduced in two fashions; namely sudden temperature increase and ramp temperature increase. The dynamic behavior of the process dependent variables, namely, the condensing temperature, evaporating temperature, and the coefficient of Performance (COP) are investigated. It is observed that the transient time that is needed for the given refrigerant to reach the new steady-state follows the following rank of refrigerants, starting with the fastest to the slowest: R410a, R32, R134a, R1234yf, and R717. Further, it is observed that the least reduction in COP upon the disturbance occurs in the chillers that run with R717, while the highest is associated with the one that has R134a.

CHT-21-106 Asymptotic properties of the radiation deep in an atmosphere, by **Menekşe Şenyiğit** and Ayşe Kaşkaş

The asymptotic light regime for polarized radiation deep within an optically semi-infinite, homogeneous atmosphere containing no interior sources is investigated using a different analytical approximation. The dependence of the asymptotic properties of the radiation on the single scattering albedo and the depolarization factor of the Rayleigh–Cabannes model is examined. The five parameters, asymptotic attenuation coefficient common to both radiation components and, for each polarization component, the outward-to-inward flux ratio and the mean cosine of the radiance, are obtained as a function of the albedo using the infinite

medium Green's function for the vector equation. It is seen that all these five parameters have a very weak dependence on the value of c for all single scattering albedo values.

CHT-21-109 The ω -absorption line distribution function for rank correlated SLW model prediction of radiative transfer in non-uniform gases, by **Frédéric André, Vladimir P. Solovjov and Brent W. Webb**

Unlike previous global methods, the recently developed Rank Correlated Spectral Line Weighted-sum-of-gray-gases (RC-SLW) model does not require specification of a reference thermodynamic state from which all other states are corrected using a correlated spectrum assumption. However, the RC-SLW approach still requires specification of an arbitrary blackbody source temperature to generate the Absorption Line Blackbody Distribution Function (ALBDF) used in construction of the spectral model. This paper reports on the development of a universal RC-SLW model that eliminates the need for the specification of a blackbody source temperature. The approach replaces the ALBDF with a new distribution function, herein termed the Omega-Absorption Line Distribution Function (Omega-ALDF), and is based on a new spectral weighting function instead of the Planck blackbody distribution function. The new weighting function is determined using the well-established ALBDF, avoiding the need to generate a radically new distribution function database from the detailed gas absorption cross-section data. The Omega-ALDF presented here depends only on the local gas thermodynamic state, and does not involve the blackbody source temperature used in the ALBDF. The Omega-ALDF-based RC-SLW model thus requires no user-specified parameters (no reference thermodynamic state and no reference blackbody source temperature). Further, only minor modification of the conventional RC-SLW model is needed to implement the new approach. Development of this new distribution function is only possible within the theoretical framework of the Rank Correlated SLW model. This work presents the theoretical development of the Omega-ALDF, and demonstrates the use and accuracy of this new universal RC-SLW model.

CHT-21-110 Stability analysis of a second order discretized 1D two-fluid model for vertical annular flow, by **R. L. Castello Branco, E. M. G. Fontalvo, I. B. de Paula, J. N. E. Carneiro and A.O. Nieckele**

A study on the stability of the set of equations for the transient one-dimensional two-fluid model resulting from a first and second order discretization scheme for vertical annular flow was performed. First order numerical scheme (upwind) introduces an excessive damping effect, which in principle may prevent growth of high frequency disturbances, such as those compatible with annular flows. In this work it is shown that the impact of the discretization order in the cut-off wave frequencies and wave growth-rates is very important. Furthermore, the inclusion of different dynamic pressure models as well as different values of the momentum flux distribution parameter in the stability analysis of the system is discussed.

CHT-21-112 Numerical simulation of a fixed bed gasifier using two fluid model (TFM), *by Massoud Massoudi Farid, Andreas Richter*

Utilization of gasification/partial oxidation technologies have been increased during the last decades due to the advantages such as flexible feedstock utilization and low carbon emission which makes the gasification a promising solution to decrease the amount of greenhouse gases emissions. Among different gasification technologies, FlexiSlag gasifier at TU Freiberg (a Fixed/Moving Bed slagging gasifier) is a promising technology to handle a variety of feedstock such as different coal ranks and coal blends with RDF/municipal waste/domestic waste, tires, and wood waste. However, technical problems such as poor interphase mixing, unreacted carbon, hot spots, and lower conversion rate in this type of reactor can significantly reduce the availability of the gasifier for a stable operation. To overcome the aforementioned problems, better understanding of different phenomena occurring inside the gasifier is necessary. In this regard, modeling tools such as computational fluid dynamics (CFD) which provides spatially and temporally resolved information of the system could be a great help. Since FlexiSlag gasifier operates near the maximum packing limit and includes a wide range of homogeneous and heterogeneous reactions, development of a comprehensive CFD model to simulate the whole process in an industrial level is a big challenge. Hence, as the first step towards the simulation of this gasifier, a simplified CFD model is developed to simulate a fixed bed gasifier using the Two Fluid Model (TFM) approach. The results are validated with the results obtained from a similar experiment and detailed temperature, pressure, and gas species distributions are presented.

CHT-21-113 Computational modeling of magnetoconvection in a laterally heated cube, *by Alexander Gelfgat and Oleg Zikanov*

The problem of natural convection in a laterally heated three-dimensional cubic cavity under the action of an externally imposed magnetic field is revisited. Flows at the Rayleigh number $Ra=10^6$ and the Hartmann number $Ha=100$, and three different orientations of the magnetic field are considered. The problem is solved using two independent numerical methods. Convergence toward grid-independent results is examined versus the grid refinement and near-wall grid stretching. Converged benchmark-quality results are obtained. It is shown that for convection flows with a strong magnetic field a very steep stretching near some of the boundaries is needed. It was found that the strongest magnetic suppression is yielded by the field directed along the imposed temperature gradient. The horizontal magnetic field perpendicular to the imposed temperature gradient stabilizes the main convection roll and leads to a flow with higher kinetic energy and heat transfer rate than in the non-magnetic case.

CHT-21-114 Convective heat transfer in open-cell foams: the effects of porosity and velocity on representative volume element size, *by Marcello Iasiello, Assunta Andreozzi, Nicola Bianco, Wilson K. S. Chiu and Vincenzo Naso*

Because of features like high heat transfer area per unit volume and tortuosity, open-cell foams are used in applications which benefit from heat transfer enhancement, such as solar receivers, heat exchangers, and thermal energy storage systems. Numerical simulations are

carried out to predict the heat transfer performance of foams, but their complex geometry makes the required computational power challenging. Therefore, the behaviour of a foam is predicted by simulations carried out on a computational domain far smaller than the volume of the foam. Reference is, then, made to a cubic sub-volume, named the Representative Volume Element (RVE), which has the same characteristics as those of the whole foam. The effects of porosity on RVEs for convective heat transfer in open-cell foams are analysed numerically in this study. Four 40 Pores Per Inch (PPI) open-cell foam samples with various nominal porosities are reconstructed by X-ray computed tomography. After building up a numerical grid with MATLAB, mass, momentum and energy equations are solved numerically with the COMSOL Multiphysics commercial finite-element code, under the assumption of uniform heat flux at the solid/fluid boundary. The interfacial convective heat transfer coefficient and volumetric heat transfer coefficient, for different nominal porosities of the foam and inlet velocities of the air, are predicted. The RVE length that minimizes the computational cost of simulations, under different nominal porosities and fluid velocities, is then determined.

CHT-21-115 Numerical simulation of Al_2O_3 -isopropanol nanofluid flows in a tube of circular cross-section, by *Pedro Romão and Pedro J. Coelho*

The development of more advanced technology with increased cooling needs and the continuous search for solutions with better energy performance have been motivating the heat transfer community to find alternatives to traditional cooling techniques. This intensive research promoted the advent of nanofluids, a type of coolant that consists of a colloidal suspension of solid nanoparticles into common cooling fluids. A numerical investigation of the heat transfer performance and hydrodynamic characteristics of Al_2O_3 -isopropanol nanofluid flows in a tube of circular cross section is reported. A single-phase approach, which assumes that the nanofluid behaves as a homogeneous fluid with modified physical properties to account for the presence of the nanoparticles, is employed. Data available from an experimental investigation is used to assess the accuracy of the predictions. Both laminar and turbulent flows are considered. A parametric analysis testing the influence of each controlling parameter considered in the experiments was conducted and the influence of the comparison basis on the interpretation of the results is discussed. A good agreement between experimental data and predictions was found for laminar flow. In turbulent flow conditions, the match between predictions and experiments was not so good, but still does not compromise the validity of the assumptions. The parametric analysis showed a small increase in the heat transfer coefficient with the addition of nanoparticles for laminar flow and a considerable deterioration for turbulent flow conditions on the basis of a constant mass flow rate. The same results expressed for a constant Reynolds number or constant pumping power produced significantly different conclusions and support previous claims that the assessment of the thermal performance of nanofluids based on constant Reynolds number is misleading.

CHT-21-117 Critical assessment of the moisture distribution in existing building walls, by *Ainagul Jumabekova, Julien Berger, Rafik Belarbi and Jean-Claude Krapez*

Current environmental issues focus on the energy performance of existing buildings. Thus, the problem of the moisture content within a wall is of capital importance. However, its

assessment in existing buildings is difficult to obtain. Therefore, the inverse problem approach is proposed. In this article the moisture distribution within the existing building wall is presented through the spatial variation. Then, the coefficients of polynomial representation are estimated using the temperature measurements. The case study of the existing building wall is considered. The obtained results and issues raised by this approach are discussed.

CHT-21-118 Real-time estimation of the heat transfer coefficient of Pitot Tubes undergoing freezing, by *Steve B. Diniz and Cesar C. Pacheco*

This paper deals with the estimation of the heat transfer coefficient at the tip of an aeronautical Pitot tube undergoing ice accretion. A new framework, very computationally efficient and based on previous works and models available in the literature is proposed, where real-time estimation of the freezing process is achieved. To do so, the typical batch estimation process is replaced by an approach in which the inverse problem is rewritten as a state estimation problem. Thus, it follows that recursive techniques can be employed. An one dimensional heat conduction model used in previous works is used as the forward problem, while the state estimation problem is solved using the Steady State Kalman filter. A good agreement between reference and estimated temperature and convective heat transfer coefficients is observed, thus demonstrating the proposed approach to be robust. The algorithm also yields a substantial reduction in computational costs now allowing for real-time estimation of the convective heat transfer coefficient, so that its application in actual flights is possible.

CHT-21-120 Transient three-dimensional conjugated heat transfer with integral transforms and single domain formulation, by *Adam H. R. Sousa, Kleber M. Lisboa, Carolina P. Naveira-Cotta and Renato M. Cotta*

In the thermal analysis of microfluidic systems, it is essential to study the conjugated conduction-convection problem due to the participation of the substrate walls in the heat transfer process, which becomes more remarkable at such scales. Thus, the present work proposes a theoretical analysis based on integral transforms for the transient three-dimensional conjugated conduction-convection heat transfer problem. The hybrid numerical-analytical approach known as the Generalized Integral Transform Technique (GITT) combined with a single domain reformulation strategy is employed, providing accurate, robust, and cost-effective simulations for determining temperature distributions and Nusselt number profiles. The fluid and solid domains are represented as one single region, where the integral transformation is carried out using an eigenvalue problem encompassing the thermophysical properties and velocity abrupt spatial variations. Converged numerical results for temperature distributions are then critically compared with a finite element solution and literature results for thermally developing laminar flow in a rectangular channel.

CHT-21-121 Modeling the process of solid fuel conversion in multi-stage gasification plants, by **A. Levin** and **A. Safarov**

This paper considers numerical modeling of heat exchange, aerodynamics, and kinetics of chemical reactions in the reactor for thermochemical conversion of wood biomass. The problem of the practical use of large volumes of fuel with low thermal efficiency of direct combustion and high oxygen content is a significant factor stimulating the development of biomass gasification technologies. A common feature of mathematical models presented in numerous studies is the joint solution of kinetic equations describing chemical transformations with the continuum equations of conservation of mass, energy, etc. Description of the chemical reactions kinetics by equations the Arrhenius type is one of the successful approaches. A detailed and complete description of the ongoing reactions is extremely challenging due to the large dimension of the system of equations. In practice, the system of equations of the chemical reactions kinetics is reduced on the basis of empirical results by decreasing the number of reactions required for consideration by an order of magnitude. For this reason, scaling the results of successfully verified models to different operating conditions (especially when changing one of the boundary conditions to make it several times bigger or smaller) and to the process plants of different size and power is extremely difficult. Therefore, mathematical models for this case are quite different from problems of numerical description of conjugated heat transfer. The prospects for active implementation of such technologies are currently limited in view of the imposed restrictions, such as the need to achieve a high degree of energy conversion; minimization of liquid and solid waste; stable operation under conditions of significant variability in the initial fuel composition. In our work, we present the results of numerical and experimental development of the technology for stepwise gasification of solid fuel.

CHT-21-124 Metal-insulator-metal selective emitter design with an emissivity matching with GaSb thermophotovoltaic cell, by **Eslem Enis Atak**, **Elif Begüm Elçioğlu** and **Tuba Okutucu-Özyurt**

A thermophotovoltaic (TPV) system converts infrared radiation to electrical energy by means of the PV effect. For a TPV system to work efficiently, the emission spectrum of its emitter must match the energy bandgap (E_g) of its TPV cell. An ideal selective emitter emits in-band photons, i.e., photons with energy, $E > E_g$ (thus $\lambda < \lambda_g$). The ways of obtaining spectral selectivity -as proposed in the literature- include employing optical filters, surface nanostructures, and plasmonic metamaterials. Recent studies showed that plasmonic resonances of metal-insulator-metal structures can be exploited to obtain very high emissivity at resonant wavelengths. GaSb with its low bandgap ($E_g = 0.72\text{eV}$, $\lambda_g = 1.72\ \mu\text{m}$) is an important receiver for modern TPV generators. Previous studies on developing selective emitters to optimally function with GaSb focused on having high emissivity at the λ_g of GaSb. On the other hand, GaSb has its highest quantum efficiency at lower wavelengths (within $1.2 - 1.6\ \mu\text{m}$) followed by a sharp decrease at wavelengths $\lambda > 1.6\ \mu\text{m}$. Tungsten (W), with high emissivity in the visible and near infrared region is a suitable TPV emitter. Metamaterial structures consisting of W (base) and SiO₂ (spacer) were also shown to be stable at high temperatures. In this work, a W-SiO₂-W nano-patterned selective emitter is proposed by performing a finite-difference time-domain analysis. Grid search optimization is used to with an objective function constructed to maximize the average emissivity up to the cut-off wavelength of quantum efficiency of GaSb, and to minimize the emissivity after the bandgap

of GaSb. The designed emitter has an average emissivity of 98.2% between 1.2-1.6 μm . At 1700 K, the ratio of in-band radiation to the total radiation emitted is calculated to be 72.3%. At the same temperature, this ratio is 27.9% for a standard SiC emitter.

CHT-21-125 Heat transfer characteristics and effective thermal conductivity for ceramic matrix composites, *by Anshul Suri and Ankit Bansal*

Porous materials have found a significant application in heat shielding and thus are used in hypersonic re-entry vehicles, rocket nozzle liners, etc., as protection from the high enthalpy flows. Porous ceramic matrix composites (CMC) are a class of materials that can be designed and manufactured in ways to have superior mechanical properties along with excellent heat-shielding properties, thus a cut above conventionally used carbon and silica phenolic. The purpose of this study is to study the heat transfer characteristics in porous CMC's, which takes place by virtue of conduction, convection, and radiation, thus creating a non-linear temperature distribution in the material. The multiple modes of heat transfer due to the porous nature of the material, and the non-linear temperature variation, set these materials apart from conventional solids. Using an inverse calculation methodology, this study analyzed the experimentally obtained thermocouple data and fitted the computationally generated, finite volume based results, using error minimization to converge and yield an Effective Thermal Conductivity (ETC) of the porous CMC. This is a novel and state of the art methodology for ETC calculation for, and not limited to, the porous CMC's, which yielded highly accurate results since the study is based on harmony between experimental and computational studies.

CHT-21-126 Onset of low-frequency shear-driven instability in differentially heated cavities, *by Krishna R. Maryada and Stuart E. Norris*

The low-frequency instability in a square differentially heated cavity at different Prandtl numbers ($0.4 \leq \text{Pr} \leq 1.4$) is investigated using two-dimensional numerical simulations. For $0.4 \leq \text{Pr} \leq 0.45$ and $0.71 \leq \text{Pr} \leq 1.4$, a low-frequency shear-driven instability in the detached flow structure bifurcates the steady flow into a periodic state. However, for $0.5 \leq \text{Pr} \leq 0.65$, this instability is observed in the unsteady regime with the flow bifurcating due to a different high-frequency boundary-layer instability. The frequency of the shear-driven instability is always less than the buoyancy frequency and excites internal waves in the stably stratified core, which re-orient themselves to form different standing internal wave modes. The standing internal wave modes govern the stability of the shear-driven instability as the instability, and internal wave modes are phase-locked in the limit cycle regime governed by this instability. The low-order internal wave modes increase the stability of the shear-driven instability and delay its onset to higher Rayleigh numbers. Feedback between the instability, stratification and the viscosity of the fluid causes a global absolute instability despite the instability being localised to the detached flow structure.

CHT-21-127 Spectral analysis on heat transfer between liquid and structured surface based on molecular dynamics, by **Kunio Fujiwara**, *Shogo Nakata and Masahiko Shibahara*

Heat transfer across solid-liquid interfaces at the nanometer scale is the important phenomenon in thermal science and engineering. This study examined effects of structures at atomic scale on heat transfer mechanisms at a solid-liquid interface, using molecular dynamics simulations. Especially, the simulations investigated the thermal transport mechanism from a spectral point of view focusing on the heat flux across a solid-liquid interface. The relationship between the thermal transport and the spectral heat flux was discussed, and the results showed that the thermal transport with low frequencies is important for understanding the thermal transport mechanism at a solid-liquid interface.

CHT-21-129 Numerical studies on the effects of different convex particle shapes and polydispersity on the heat transfer in Fixed Beds, by **Shreyas Rohit Srinivas**, *Massoud Massoudi Farid, Andreas Richter*

The FlexiSlag fixed bed gasifier at TU Freiberg has the potential to gasify coal and waste materials. Polydisperse coal and waste particles with different shapes undergo a number of chemical processes inside the gasifier where the heat transfer between the particles and gas plays a vital role. Heat transfer and interstitial flow in a fixed bed depends strongly on the local porosity distribution which is a function of shape and size of the particles. Hence, investigation of the effects of particle shapes and polydispersity on heat transfer in fixed beds is crucial for optimization and upscaling of the FlexiSlag gasifier. In this study the effects of a few regular particle shapes, like ellipsoidal, cylindrical, and spherical on the heat transfer at two different computational scales are numerically investigated. A DNS model is used to study in detail the influence of particle shapes on interstitial flows and local heat transfer and modifying the heat transfer correlations to include the effects of particle shapes. Modified correlations are tested using coupled CFD-DEM simulations to achieve a better understanding of the heat transfer in a fixed bed. For the DNS simulations a bed geometry is generated from Stereo Lithographic (STL) geometries of the particle shapes, while for the coupled CFD-DEM simulations glued sphere model is used to represent different particle shapes. The heat transfer in the bed is validated with experimental data for cylindrical particle shapes and the effects of other particle shapes on the heat transfer are studied numerically.

CHT-21-130 Thermal performances of cross-flow microchannel heat sinks, by **Carlo Nonino** and *Stefano Savino*

A numerical investigation is carried out that shows how reasonably good thermal performances can be obtained with cross-flow microchannel heat sinks provided that an unequal number of microchannels is used in the two layers and a non-uniform microchannel inlet velocity distribution is produced by properly designed headers. All the numerical simulations are carried out using an in-house FEM procedure which solves the parabolized form of the Navier-Stokes equations in a computational domain corresponding to a single microchannel. Then the velocity field thus obtained is appropriately scaled and mapped onto the fluid parts of the 3-D domain corresponding to the whole microchannel heat sink, where the elliptic form of the energy equation is solved.

CHT-21-131 Particle filter-model predictive control for oil reservoir management, by **Carlos Eduardo Rambalducci Dalla**, *Tarsis Baia Fortunato, Julio Cesar Sampaio Dutra, Wellington Betencurte da Silva, Jose Mir Justino da Costa and Marcelo José Colaço*

In this work, the application of a Nonlinear Model Predictive Control (NMPC) with state estimation in the waterflooding process as supervisory control was studied. The methodology employed the Particle Filter (PF) in step of the model-based optimization of the NMPC with Particle Filter Optimization (PFO) and step of the filtering through the Auxiliary Particle Filter (APF). This way, it is presented a new Bayesian approach to NMPC for reservoir management. The proposed methodology aimed at being robust to overwhelm nonlinearities and non-Gaussian uncertainties inherent in oil reservoir systems. The results showed the potential of APF in the estimation step not presenting degeneration or impoverishment of the sample, in view of that the dimension of the problem is considerably high, and, in the model-based optimization step with PFO which handled well the nonlinearity of the model and maintained control of production. The results also supported the contribution of this work with advances in the application of PF as a tool in the context of reservoir management and especially in its use as an optimization tool.

CHT-21-132 Computational study of natural convection flow in an open-ended channel coupled with a room: application to building-integrated photovoltaic (BIPV) systems, by **S. Tkachenko**, *H. Ahmadi Moghaddam, J. Reizes, R. Raja, C. Menezo, S. Giroux-Julien and V. Timchenko*

Many investigations have focused on the performance assessment of building-integrated photovoltaic systems as a renewable and clean energy resource. A major problem with photovoltaic panels is that their electrical performance decreases with an increase of their temperature. The natural convective flow generated in the space between PV panels and the building's outer surface, as a passive cooling method, could be used to improve their performance. At the same time, the generated flow could be utilized for the ventilation of indoor environments. The current numerical research evaluates a natural convection flow generated in an open-ended channel coupled with a room which replicates a solar chimney system. The effects of various factors are studied such as heat flux applied on the chimney walls, the number of chimney heated walls, the emissivity of the chimney walls, and the configuration of windows in the room. For this purpose, a 3D computational fluid dynamics model has been developed using Ansys Fluent software. The shear-stress transport turbulence model has been utilized as the turbulence model. The radiation effect was simulated using the surface-to-surface radiation model. It was found that, for any heat flux, two heated walls mode generated a larger buoyancy-driven mass flux than the single heated wall mode while the total applied heat flux for both cases was equal. It was also observed that an increase in the emissivity of the surfaces of the chimney resulted in the rise of the convective mass flow rate and enhancement of the cooling effect on the heated walls. Increasing the emissivity of walls from 0.1 to 0.95, depending on the heating mode and applied heat flux, yielded the maximum increase of 61% in the buoyancy-driven mass flow rate with correspondent decrease of 10% in the maximum temperature of the chimney walls. It was observed that the position of windows in a room affects the natural convective flow in the room and the induced mass flow rate in the channel.

CHT-21-133 Enhancement of the RC-SLW model for prediction of gas radiation in non-uniform media, by *Brent W. Webb, Vladimir P. Solovjov and Frédéric André*

The choice of gray gas absorption coefficient in the Rank Correlated Spectral Line Weighted-sum-of-gray-gases (RC-SLW) model is investigated. Several options are considered for specifying the gray gas absorption cross-section from the bounding supplemental absorption cross-sections, including that determined by inversion of the F-variable using Gauss Quadratures, the Geometric Mean of the bounding values, the Arithmetic Mean, and finally, a value determined from the weighting of the bounding supplemental absorption cross-sections using a variable f . It is shown that an optimal value of the gray gas absorption coefficient can only be determined by accounting for the path length L . However, test cases and theoretical confirmation reveal that the Geometric Mean of the bounding supplemental absorption cross-sections for the gray gas absorption coefficient is the preferred method.

CHT-21-134 The adaptive PLIC-VOF method in cavitating flow simulations, by *Dezhi Dai and Albert Y. Tong*

Piecewise Linear Interface Calculation (PLIC) schemes have been extensively employed in the Volume of Fluid (VOF) method for interface capturing in numerical simulations of multiphase flows without phase changes. The Adaptive Mesh Refinement (AMR) is often adopted to increase the local mesh resolution dynamically within the cells which contain the interface. Cavitation appears when local static pressure drops below the water vapor pressure and usually causes significant impacts on hydraulic devices. A PLIC-VOF method with AMR has been adopted to capture the interface between liquid and vapor phases in cavitating flows. A modified version of the Schnerr-Sauer cavitation model has been used to compute the local mass transport rate for the vaporization and condensation processes. Turbulent eddy viscosity is evaluated by using the Large Eddy Simulation (LES) technique. Simulations are performed under the framework of OpenFOAM with a modified flow solver. Numerical simulations of cavitating flows around an axisymmetric hemispherical structure have been successfully performed using the adaptive PLIC-VOF method. The findings in the present study are consistent with experimental studies reported in the literature.

CHT-21-135 Molecular dynamic study of local interfacial thermal resistance of solid-liquid and solid-solid interfaces: water and nanotextured surface, by *Yoshitaka Ueki, Satoshi Matsuo and Masahiko Shibahara*

Degradation in the performances of air conditioners and refrigerators is caused by frost formation and adhesion on the surface. In the present study, by means of the classical molecular dynamics simulation, we investigate how and how much the nanotextured surface characteristics, such as surface wettability and geometry, influenced the interfacial thermal resistance (ITR) between the solid wall and the water/ice. The local ITR was relatively high at the nanostructure bottom corner and low at the nanostructure top corner when the H₂O molecules were in the water state. In the ice state, the local ITR was influenced by the ice structure neighboring the Pt solid wall. Especially when the H₂O molecules were in the crystal form, the local ITR significantly increased.

CHT-21-137 Heat transfer through shadowed droplets in dropwise condensation, *by George Memos, George Kokkoris, Vassilios Constantoudis, Athanassios Milionis, Dimos Poulidakos, Evangelos Gogolides*

Dropwise condensation (DWC) in lieu of filmwise condensation ensures efficient heat transfer and enhances the performance of related devices. The efficiency of heat transfer in DWC depends on the heat transfer rate through a single droplet and the droplet-size distribution. While the former can be captured through the thermal resistance model, the theoretical analysis of the droplet-size distribution involves assumptions oversimplifying the complexity of droplet interactions, especially in the sub-10 μm regime. Here, we adopt a computational approach to accurately predict the droplet-size distribution in the whole size range, simulating the entire droplet life-cycle from nucleation to departure, either by coalescence induced jumping or gravity sweeping, and treating condensing droplets as interacting 3d entities. Although larger droplets can be easily observed in experiments, our work shows that the large droplets do not significantly affect heat transfer on superhydrophobic (SHB) surfaces. Instead, it is the small (with radius $< 10 \mu\text{m}$) “shadowed” droplets, i.e. the droplets grown in the shadow of the large ones, that play the dominant role in heat transfer. Due to the growth of these droplets, the shift in the droplet size distribution towards smaller sizes is significant enough to keep heat transfer rate nearly insensitive to the presence of large droplets. Through comparison with measurements of the heat transfer coefficient on SHB surfaces, the critical role of the density and the distribution of the nucleation sites on the heat transfer is deduced.

CHT-21-138 Numerical solving of geometry-radiative inverse problem, *by Aleksey V. Nenarokomov, Evgeny V. Chebakov and Dmitry L. Reviznikov*

A reliable control of current orientation of a spacecraft is a critical task in aerospace engineering, as the loss of the spacecraft attitude can endanger the whole mission. This makes important to elaborate a reliable and robust attitude control system of a spacecraft, which can extend its lifetime. In order to develop it we use various conditions of radiative heating at the surface of spacecraft’s elements with different directions to the Sun and a planet which a satellite orbits to estimate their angular position. In the case of slow angular velocity of a spacecraft, temperature measurements can be used to estimate integral (over the spectrum) radiative flux to various surfaces of specially designed thermal sensors at different convex surfaces of the spacecraft. Then estimated heat fluxes can be used to determine attitude of the spacecraft. To provide this approach it is required to consider one of the so-called inverse heat transfer problems, which is mathematically ill-posed and therefore rather challenging. Thus, the authors aim to solve this ill-posed problem. The traditional methods of the inverse problems regularization are modified to take into account special features of the heat transfer problems under consideration. In order to estimate the spacecraft’s attitude during spaceflight the suggested approach was supplemented by the Kalman filter.

CHT-21-142 Numerical analysis of a MHD generator with helical geometry, by **Tomas S. Quirino, Gabriel L. Verissimo and Marcelo J. Colaço**

In this study, three-dimensional steady-state numerical simulations of a helical-channel MHD generator coupled with an outer resistance circuit are conducted. Generator design consists of a circular pipe made of conducting walls, combined with an inner helical insulation wall and an external solenoid magnet that produces a uniform magnetic field in the axial direction. The numerical model comprises the typical mass and momentum conservation equations for incompressible Newtonian fluids, including also the Lorentz force due to the magnetic field. An additional equation for electric charge conservation closes the system. An iterative algorithm is used for coupling the mathematical models for the generator and the outer circuit, assuring that the Ohm's and Kirchhoff's Law are obeyed within a predefined accuracy level. The computational model is validated against experimental results obtained in the literature. Simulation results for the helical-type generator allow the evaluation of its performance characteristics, including output power and efficiency. Then, the helical geometry that maximizes the electric power produced by the MHD generator is identified, as the geometry with the highest MHD generator efficiency.

CHT-21-143 Estimation of thermal contact conductances between different materials by the reciprocity functional using heat flux and transient temperature measurements, by **Inoussa Tougri, Luiz Abreu and Marcelo Colaço**

The thermal contact conductance knowledge on the contacting interface between two bodies made of different materials is of great importance in engineering applications. In this work we use the reciprocity functional method, a non-iterative and non-intrusive technique, to estimate this quantity. The main difference between this and our previous works is the fact that, in this paper a constant heat flux is applied on one side of the material and a transient temperature data is measured on the other side, while in our previous works both quantities were evaluated on the same side of the material. These two quantities are used for the solution of an inverse problem. The reciprocity functional requires the formulation of an auxiliary problem for each function to be estimated and the establishment of orthonormal functions that will serve to assemble a base system. Through an appropriate choice of the orthonormal basis and using the analytical solution of the auxiliary problems, it is possible to reduce the solution of the inverse problem to a simple algebraic equation. The method was verified using synthetic measurements and validated with experimental measurements obtained through a thermography camera.

CHT-21-144 Design under uncertainties of the thermal ablation of tumors with high-intensity focused ultrasound, by **Rodrigo L. S. Silva, Mohsen Alaeian and Helcio R. B. Orlande**

In clinical applications, thermal ablation consists of the removal or destruction of a specific tissue by heat. High Intensity Focused Ultrasound (HIFU) is a non-invasive technique that can be used for the thermal ablation of tumors with minimum side-effects. This work dealt with the design of thermal ablation of a tumor heated by HIFU. A two dimensional region with a hypothetical rectangular tumor was considered here. The acoustic problem was simulated with the numerical solution of the mass and momentum conservation equations. The heating

process was optimally designed under uncertainties in the model parameters by using the Markov Chain Monte Carlo method, implemented via the Metropolis-Hastings algorithm. Two design variables were considered in this preliminary work, namely: the heating time and the vertical location of the HIFU transducer. The obtained results revealed that the Metropolis-Hastings algorithm could deal with all associated uncertainties and provided a robust design for the problem under analysis.

CHT-21-145 Thermal transport within porous biological tissue for thermal therapeutics, *by Amit Kumar Shaw and Sanjeev Soni*

During thermal based cancer therapeutics, it is very important to estimate the thermal transport to predict the resulting tissue temperature. Higher temperature causes damage to the cancerous tissues as well as healthy tissue, so it is clinically important to quantify the spatiotemporal temperature to minimize the damage to healthy tissue. Estimation of thermal transport within biological tissue is challenging due to the presence of complex vasculature. Several researchers have developed mathematical models to quantify the temperature field. In this paper, a porous media based bioheat model is used to obtain the temperature distribution for a 3D tumor-tissue domain. Porous media accounts for the local vasculature effects as well as tumor physiology like porosity etc. The direction as well as magnitude of local blood flow significantly affects the temperature distribution. So, the effect of blood parameters viz. blood flow direction, local blood velocity is computed. Also, the effect of tumor porosity is evaluated considering external heat sources applied over the tumor surface. The influence of these parameters is very much required for pre-treatment planning for such thermal therapeutics. Higher external heat flux applied over the surface results in deeper contour region but higher blood flow through tissue achieved by higher local blood velocity and/or higher porosity caused increased or decreased temperature contour of 43°C within the biological tissue depending upon the direction of blood flow.

CHT-21-154 Approximate semi-analytical method for solving of diffusion problems with variable properties, *by Isabela Florindo Pinheiro and Leandro Alcoforado Sphaier*

This paper proposes an alternative semi-analytical methodology for the computational solution of diffusion problems with variable thermal properties. The method itself involves approximating the variable property coefficients within sub-domains, in which the approximate diffusion equations are then solved analytically, leading to an algebraic system for determining coupling coefficients. Both time-dependent problems or steady state diffusion are considered. The solution scheme is illustrated by a general formulation considering different regimes and different properties in conduction heat transfer problems. The presented formulation is imposed to differential equations with similar form to what is encountered during the implementation of the Generalized Integral Transform Technique (GITT). Two test-cases of diffusion problems are selected to show the viability of the method, based on the resulting transformed ordinary differential equations at the final step of the GITT procedure, where the thermal properties are dependent of spatial coordinates or time. The numerical results obtained in both steady and transient regimes are then compared (and verified) with a traditional finite-difference scheme. As shown in the results, the considered method produces good agreement between approaches.

CHT-21-155 Numerical analysis of explosive solidification under the effect of different boundary conditions, by **Çiğdem Susantez, Bruna R. Loiola and Aldélio B. Caldeira**

Casting of explosives in a shaped charge shell for the production of warheads and anti-tank ammunitions is an important process. This type of device has a conical void coated by a metal liner, which promotes a high velocity jet of the liquid metal after the detonation of the explosive. Distinct explosives are employed with this purpose and an investigation of the cooling conditions is suitable. Therefore, the objective of this work is to evaluate numerically the solidification process of TNT, Baratol and Composition B explosives inside a shaped charge by utilizing the apparent heat capacity method on a transient-diffusive heat transfer equation to model the phase change. The mathematical model is solved in COMSOL Multiphysics and Modeling Software by a finite-element approach. The solutions are verified against literature ones. Prescribed temperatures are considered for conical and bottom surfaces, while natural convection is applied for the outer surfaces. Three boundary conditions for top surface, namely convection, adiabatic and isothermal boundary conditions are analyzed in the simulations. Results show that, for the same analyzed geometry, Baratol has solidified in less time than TNT and Composition B. It has been concluded that the most sensitive parameters of this process are the thermophysical properties of the explosive. Finally, the isothermal top boundary condition showed to be preferable to promote solidification of high explosives in shaped charge shell.

CHT-21-157 A thermochemical energy storage reactor model – code formulation, verification, and experimental validation, by **Michael Wild and Aldo Steinfeld**

We report on the design and modelling of a novel thermochemical energy storage (TCS) reactor which makes use of reversible gas-solid reactions in a tubular packed bed with radial flow to store heat at high temperatures. The calcination/carbonation of limestone ($\text{CaCO}_3 \leftrightarrow \text{CaO} + \text{CO}_2$) is selected as the endothermic/exothermic thermochemical reaction. A 1D two-phase model of the TCS reactor is formulated to resolve the gas flow and heat transfer via conduction, convection and radiation, coupled to the chemical reaction rates. Temperature-dependent material properties are implemented. Reaction rates are dynamically prescribed by either local equilibrium conditions or kinetics determined by thermogravimetry. The governing conservation equations are numerically solved by the finite-volume technique and verified using the method of manufactured solutions and grid refinement. The implementation of an adaptive time-step generic Runge-Kutta time-stepper and its verification using the example of the 3rd-order Bogacki-Shampine Method is presented. The TCS reactor model is validated using experimental data obtained with a lab-scale reactor prototype in terms of the temperature distribution across the packed bed and the CO_2 evolution/consumption, which were measured as a function of time for multiple consecutive calcination/carbonation cycles. The corresponding volumetric and gravimetric energy densities of 203.4 MJ/m³ and 880.7 kJ/kg were determined. The validated model serves as a tool for optimization and scale-up of the TCS reactor.

CHT-21-158 Identification of impulse responses in heat transfer: Dirac comb parameterization, cumulated doses and partial time moments, by **Denis Maillet** and **Benjamin Rémy**

When thermal diffusion and possibly fluid advection occur in a material system, the transient temperature response in one point is a convolution product between an impulse response and a thermal source (heat power or temperature). Three conditions are required: i) the heat transfer model is Linear with Time Invariant coefficients, ii) the transient source is unique and separable and iii) a pre-existing steady state thermal regime takes place, without necessarily being a uniform one. If discrete and exact observations of the source and of the temperature response are available, the corresponding impulse response can theoretically be retrieved using a deconvolution algorithm. It is independent from the source and can be seen as the identity card of the system. However, in a real calibration experiment, both signals are corrupted by noise and the experimental deconvolution constitutes an inverse problem of the identification type, which is ill-posed. So, some kind of regularization such as Tikhonov regularization for example, is required, in order to get a stable impulse response, with however presence of some bias. Here, another approach is explored. It is based i) on a parameterization of the three functions involved by projection onto a Dirac comb basis, ii) on the use of their cumulated doses to find the time support where the impulse response can be sought, iii) on the use of their partial and scaled time moments as observable quantities in a linear inversion procedure. This one can be implemented using a isochronous or a non-isochronous time step expansion for the parsimonious model that has to be inverted. The effect of noise of the input and output is not taken into account yet.

CHT-21-161 Numerical analysis of radiofrequency ablation in a tumour tissue bounded by healthy tissue, by **Claudio Tucci**, **Macarena Trujillo**, **Enrique Berjano**, **Marcello Iasiello**, **Assunta Andreozzi** and **Giuseppe Peter Vanoli**

Medical interest in thermoablation of tumours is growing more and more throughout the years, because it is a minimally invasive treatment which yields few complications, a short hospital stay and low costs. The interest of the thermoablation is to destroy completely the tumour without further recurrence and save the surrounding healthy tissue from the high temperatures. Computer modelling of the specific treatment has a key role in predicting effectiveness of the technique since it allows to compute the coagulation zone and temperature profiles in tumour tissues. In this study we focus on a computer model for a 12-min radiofrequency ablation (RFA) of in vivo liver tissue using a cooled electrode. The model is based on the porous media approach and employs a Local Thermal Non-Equilibrium (LTNE) equations modified in order to take into account the vaporization of water in the two phases (tissue and blood). The LTNE equations are applied separately in two different cases: healthy liver tissue and a tumoral tissue surrounded by healthy tissue. Governing equations with the appropriate boundary conditions are solved with the finite-element code COMSOL Multiphysics®. The results are presented in terms of coagulation zones transverse diameters and temperature fields obtained at the end of the application. Furthermore, temperature evolution in three different points during the 12-min ablation is evaluated. The outcomes show relevant differences when the tumour is included in the model. Thus, the different electrical conductivity and thermal properties between the two types of tissues play a fundamental role in the outcomes.

CHT-21-163 A concise and accurate solution for radiative transfer problems relevant in hyperthermia models, by **Fernando Groff, Liliane Basso Barichello and Esequia Sauter**

In this work, the Analytical Discrete Ordinates method is used to derive solutions for a radiative transfer problem relevant in simulations for hyperthermia therapy. A reformulation of the problem is proposed to deal with the singular component of the solution, due to the laser effect. A multislabs geometry is considered to represent a medium with nonhomogeneous properties and an analytical solution in terms of the spatial variable is developed for a model with boundary conditions that include diffuse and specular reflection. Simulations are performed in order to analyze the laser effects, the scattering in the medium as well as its optical thickness. The ADO solution is concise, accurate and fast. Numerical results indicate the relevance of using higher order approximations of the radiative transfer equation to properly simulate problems in this area.

CHT-21-165 Thermal and fluid dynamic behaviors of a slightly horizontal ventilated roof under variable climatic condition, by **Bernardo Buonomo, Lucia Capasso, Oronzio Manca and Sergio Nardini**

One of the European Directive priorities is represented by the improvement of “building performance requirements” and the development of new strategies for “very low energy buildings”. The goal is the reduction of the energy consumptions due to the heat flux transmitted through the envelope of residential and commercial buildings. In regions, like Mediterranean region object of this study, with high level of solar radiation ventilation allows to the cooling load during summer period and contributes to the reduction of the energy needs of buildings. The most important advantage is the reduction of the heat fluxes transmitted by the structures exposed to the solar radiation, thanks to the combined effect of the surfaces shading and of the heat removed by the air flow rate within the ventilated air gap. This paper illustrates a numerical investigation on the effect of a slight inclination angle of a prototypal ventilated roof for residential use site in Aversa (Italy). The system is studied considering a roof with a length equal to 6.0 m and three different inclination with respect to the horizontal plane (0° , 2° , 5°). The ventilated channel, under the roof, has a height of 10 cm. The analysis is carried out on a two-dimensional model in air flow and the governing equations are given in terms of k - ϵ turbulence model. The investigation is performed to evaluate thermal and fluid-dynamic behaviors of the ventilated roof as a function of the different conditions applied on the top wall and the bottom wall of the roof in summer and winter regimes. Different values of heat fluxes are applied on the top wall of the ventilated cavity, whereas through the bottom wall there is a heat transfer toward an ambient by means a thermal conductance. Moreover, the upper surface of the ventilated roof exchange heat with the external ambient. The problem is solved by means of the commercial code Ansys-Fluent. Results are given in terms of temperature and pressure distributions, air velocity and temperature profiles and show a better performance of the system when increase the inclination of the pitched roof, especially in velocity values with an increase of 0.40 m/s.

CHT-21-167 Optimized design of phase change packed beds, by **Carlos E.L. Nobrega and Sérgio L. Braga**

Thermal energy storage systems are becoming more frequently applied in HVAC installations to promote an efficient management of chiller operation. The usual design is to store as much

energy as the corresponding demand during the grid peak period. Phase change units are particularly attractive due to the high density of energy storage. The dynamical behavior of such units has been simulated by solving a mathematical model, which considers the fluid temperature field across the unit length and the phase change in the spherical capsules. Accordingly, the thermal storage unit is represented by a phase change porous media submitted to a uniform flow. The physical domain is discretized using the finite volume technique, with the latent heat release represented by a heat source as a function of position. The phase change evolution inside the spheres is represented by a quasi-stationary model. The present work addresses the optimal fragmentation of the phase change media regarding the amount of time required to charge the unit.

CHT-21-168 Estimation of thermal contact conductance on irregular interfaces using the reciprocity functional approach, *by Guilherme C. de Freitas and Marcelo J. Colaço*

In some industry applications, such as evaluation of the quality of contact between material bodies, or identification of discontinuities or cracks inside a homogeneous body, it is required the estimation of a thermophysical parameter known as thermal contact conductance. In order to calculate this parameter, one has to determine the distribution of temperature discontinuities along the contact surface, as well as the heat flux across that surface; the ratio of these two parameters gives the desired thermal contact conductance. However, the task of estimating those parameters presents difficulties because the methods employed may demand direct measurements, usually obtained by intrusive means; or they may demand a detailed description of the surfaces in contact, which is not always available. Several strategies have been developed, eventually falling into either of the features just described. Recently, some works conducted by our group have been able to address these issues by applying the Reciprocity Functional approach, leading to a non-intrusive and non-iterative method for estimation of the thermal contact conductance. In this approach, a set of auxiliary problems are introduced and their solutions are used to assemble closed-form expressions for estimating the temperature discontinuities and heat flux across the contact interface. This method has been successfully employed in the estimation of thermal contact conductances along planar contact interfaces inside composites having a rectangular cross-section. This paper aims to extend the application of the Reciprocity Functionals to a more general class of problems, in which the contact interfaces have arbitrary, non-regular shapes, being the planar contact interface a particular case. The results obtained show how this approach is capable of recovering the distributions of temperature discontinuities and heat flow across the contact interface in a fast and effective fashion. This paper also presents a stopping criteria for the summation series developed in the method, which provide the aforementioned quantities. The influence of the uncertainty in the location of the contact interface is also analyzed in this paper.

CHT-21-169 Numerical study of a wing section with a tangential blowing jet control system, *by Bruno Goffert, Ricardo Galdino da Silva, Cayo Prado Fernandes Francisco, Evgeny Pigusov, Chuang Wei, Zhansen Qian, Maria Luísa Collucci da Costa Reis*

Systems for enhancing aerodynamic lifting by blowing air over wings are used in Short Take-off and Landing (STOL) aircraft. The purpose of this paper is to compare experimental and

numerical results of aerodynamic loads acting on the RAE 102 wing section equipped with an internal duct from which the air jet is blown to a spanwise slot. The baseline airfoil and combinations of flap and slat deployments with steady blowing jet applications were investigated in the two-dimensional analysis. Three RANS codes, including the open source SU2 code, CFD++ and the in-house ARI_Overset code from AVIC ARI were used for the comparisons of the numerical solutions. Spalart-Allmaras and Menter's Shear Stress Transport turbulence models, along with structured and hybrid meshes were considered in this study. All cases were simulated for Mach number 0.132 and Reynolds number 3.78×10^6 , where the discrepancies between results are quantified by relative errors. The reference values are experimental data extracted from specialized literature. Significant differences of lift coefficient were observed between the numerical codes and turbulence models. Suppression of the flow separation, lift augmentation and drag reduction due to the blowing employment are reported.

CHT-21-170 Particle-laden multiphase flows: a finite element analysis on biofuel particle emissions, by *Joao P. I. Souza and Gustavo R. Anjos*

Particle-laden multiphase flow is an important subject of study in fluid mechanics, especially in the oil and gas industry. In this work, the particle emission from biofuel production is analyzed and simulated, in order to obtain the main effects of such transportation into the atmosphere, that may cause environmental and health damages. The continuous phase is numerically simulated directly through the Navier-Stokes equations, for which the results are in complete accordance to the ones presented in the literature. As for the solid dispersion, an Euler-Lagrange analysis is made, which provides a better understanding of each particle trajectory. A numerical simulator is built by means of The Finite Element Method (FEM) and the results are generated for different meshes, which are made for different geometries. All the results and comparisons are shown and discussed throughout this article.

CHT-21-171 Decoupled mesh method for finite element simulation of two-phase systems, by *Daniel B. V. Santos and Gustavo R. Anjos*

This paper describes a finite element solution for a two-phase flow problem, where the fluid mesh and the interface mesh are decoupled. One single phase example is shown to validate the finite element code, and two two-phase flow examples are presented, the static droplet and the oscillating droplet, with air and water as fluids. Examples work as expected and show that the methodology is valid and suitable for two-phase flows.

CHT-21-175 Heat transfer dissipation estimation in extrusion processes, by *Carlos E. L. Nóbrega*

Extrusion is a process of utmost importance in metal, polymeric products and optical fiber manufacturing, to name a few. The extrusion process is often followed by a "heat treatment". Accordingly, the mathematical modeling of thermal transport in extrusion has been addressed by a number of studies. The classical modeling of this problem leads to a non-homogeneous linear second order boundary value problem, which can be easily solved by using the Laplace Transform. The existence of an analytical solution allows for the Jacobian matrix to be also

analytically determined, which benefits accuracy and significantly mitigates the computational effort. However, the Jacobian matrix shows to be dependent on the parameter vector, which characterizes the inverse problem as non-linear. The experimental data is obtained using a “simulated experiment”, by adding a random noise to the output data generated by the mathematical model with pre-set value for the parameter vector P . This data plays the role of experimental data, and is used by the inverse problem methodology to retrieve the values of the parameter vector. The procedure uses the Conjugate Gradient method to minimize the norm, which is comprised by the squared sum of the difference between the solution and the experimental data arrays. The results show the two heat transfer parameters can be retrieved, using only a few temperature measurements along the domain.

CHT-21-176 Influence of solving the wall-region on heat transfer over a circular cylinder in crossflow, *by Gabriel Rodrigues de Oliveira Anuniação and Tânia Suaiden Klein*

Accurate prediction of heat transfer in a circular cylinder in crossflow is of great interest to the industry, given its wide applicability. While scale-resolving approaches can return accurate predictions, they are computationally expensive. RANS approaches are, therefore, still useful to allow reasonable results at a low or moderate computational cost. When it comes to heat transfer, the wall region is of great importance. The present work assesses the influence of solving the wall-region on predicting heat transfer in a circular cylinder in crossflow at different Reynolds numbers and turbulence intensities, since this is not systematically discussed in the literature. The study is carried out by comparing the standard $k-\epsilon$ turbulence model with wall function and the SST turbulence model, taking into account grid requirements for each scheme. Results are compared with experimental data and show that local Nusselt number can only be captured if the wall-region is properly solved.

CHT-21-178 Soot prediction in flames using a data-based machine learning approach, *by Joseph N. Squeo and Xinyu Zhao*

Soot prediction in combustion systems remains a challenge due to the underlying complex physical processes and uncertainties in model parameters. Collecting experimental data of flames is costly with accurate measurements and often difficult to obtain for large-scale pool fires. Models of flames that provide accurate soot prediction for sufficiently accurate radiative heat transfer prediction are an efficient means to improve fire prediction and improve our understanding of fire dynamics. Following the wake of machine learning (ML) algorithms development, data from well-validated computational fluid dynamics can be used to predict soot in flames using key parameters relating to combustion. Machine learning includes data-based algorithms that involve training a model to predict an outcome. In this work, a Poisson supervised regression machine learning model is trained using several key soot-related parameters from five chemical mechanisms and tested on data from one additional chemical mechanism for an atmospheric, 1D premixed ethylene and air flame first. The methodology is extended to a well-validated dataset of a 2D atmospheric laminar diffusion flame on the Santoro burner and tested on a similar flame with modified flow conditions. The trained machine learning model is capable of predicting the location of the entire soot field with sufficiently accurate prediction of the concentration of soot.

CHT-21-179 A comparison of two approaches to extend nodal integral methods for heat and mass transfer to arbitrary geometries, by *Ibrahim Jarrah, Sundar Namala and Rizwan-uddin*

Nodal Integral Methods (NIM) are a class of coarse-mesh numerical methods developed to solve partial differential equations (PDEs). They are more accurate and efficient compared to the conventional finite-difference, finite-volume, and finite-element methods, because of the use of approximate analytical solutions to the governing differential equations in the development of the scheme. The transverse integration process, which reduces the PDE into a set of ODEs, restricts the application of NIM to domains discretized by rectangular elements in 2D and cuboid elements in 3D. Two approaches presented in this paper relax this restriction and extend NIM's efficiency to arbitrary geometries in 3D. In the first approach, NIM is derived in general 3D curvilinear coordinates, and applied to domains discretized by hexahedral elements. The hexahedral elements in the Cartesian system are transformed into cubes in curvilinear coordinates, where the transverse integration procedure can be applied. The second approach is a hybrid nodal-integral/finite-element approach. In this approach, the bulk of the domain is discretized into regular cuboid elements, and the regions adjacent to curve boundaries are discretized by tetrahedral elements. The standard NIM is applied to the cuboid elements, while the finite-element is used for the tetrahedral elements. Both approaches are used to solve the 3D convection-diffusion equation on two domains in this paper. The first is a cylindrical annulus domain, and the other is a cylindrical domain. Numerical results of the two approaches are presented. The accuracy and efficiency of both methods are compared.

CHT-21-181 CFD analysis of the thermal performance of a Trombe wall, by *Afef Laribi, Yacine Ait-Oumeziane, Valérie Lepiller, Sylvie Begot and Philippe Desevaux*

The building sector is a huge energy consumer in the world, and particularly in France, mainly because of the need to supply inner climatic comfort conditions. Passive solar systems present effective means to decrease the energy needs by using renewable sources. Among these different systems, Trombe walls are one of the most attractive solutions due to their simple design and their capacities to achieve energy efficient buildings. A Trombe wall is a south-facing system composed of an outside glass panel separated from an inside opaque storage wall (massive wall) by an air layer. In order to allow connection between the air layer and the room, vents are present on the upper and the lower parts of the storage wall to promote convective heat exchanges. Its integration into the building aims to enhance solar radiation by combining two physical phenomena: the greenhouse effect through glazing in the air layer and the thermal inertia of the wall. However, this system has drawbacks such as overheating in summer conditions. Therefore, adjustments must be considered aiming to adapt the system performance regardless of weather conditions. Our study consists in developing a numerical model in order to simulate the thermal behavior of a Trombe wall. The steady-state behavior of the Trombe wall is studied using a two dimensional CFD model simulating the air flow and heat transfer in a Trombe wall coupled to a room. The CFD model of the system is checked and validated in comparison with experimental studies from the literature. A parametric study concerning the influence of the vents size and the air gap depth is led. The thermal performance of the Trombe wall are numerically investigated using several parameters

(temperatures and velocities) describing the thermo-aeraulic aspects and through the thermal efficiency of the system.

CHT-21-183 Numerical studies on underexpanded jet flows using commercial and open source CFD packages, by *Jonathan Ribeiro Martins, João Victor Barbosa, Luiz Fernando Lopes Rodrigues Silva, Fabio Pereira dos Santos*

Flammable Gases leaks at high pressures are hazardous, especially the free underexpanded jets. Due to the difficulty to obtain experimental data from this jets, related to the incredible speeds and gradients, Computational Fluid Dynamics (CFD) has become an essential tool. In this work, we performed simulations for free underexpanded jets to identify algorithms that better represent this type of problem. To study different algorithms, two software were used: OpenFOAM and ANSYS Fluent. Our study concluded that all algorithms and software had a satisfactory result with close experimental data results. However, we observed that Fluent had a considerable advantage because the simulation was faster compared with other solvers in OpenFOAM.

CHT-21-184 Coupled Monte Carlo-CFD model of a solar air receiver for high-temperature industrial processing, by *Vikas R. Patil and Aldo Steinfeld*

Concentrating solar thermal technology offers a clean source of process heat for high-temperature ($>1000\text{ }^{\circ}\text{C}$), energy-intensive industrial processes such as production of metals and cement, solid waste recycling, and the thermochemical synthesis of transportation fuels. Air receivers, employing porous ceramic structures as volumetric absorbers of concentrated solar radiation and air as the heat transfer fluid, have been shown to deliver high-temperature process heat. We report on the computational modeling and experimental testing of a 5 kWth air receiver comprising a cavity lined with reticulated porous ceramic (RPC) structures as absorbers. To study the inter-related transport phenomena, the Monte Carlo (MC) ray-tracing method was implemented to solve radiation exchange across the RPC, treated as a non-gray, scattering-absorbing-emitting medium. The MC solver yields the energy source term for each discrete volume of the RPC domain, which is further used in a commercial computational fluid dynamics (CFD) code to solve the Navier-Stokes equations, yielding temperature and fluid flow fields. The energy source term in the MC solution depends on the temperature of thermal emission of RPC, which in turn is determined by the CFD solution, forming an iterative algorithm that is run until temperatures converge. A prototype of the air receiver was fabricated and tested under high-flux thermal radiation to experimentally validate the coupled MC-CFD model. The validated model is applied to optimize the receiver performance for maximum solar-to-heat conversion efficiency and to perform a scale-up study for a solar tower implementation.

CHT-21-185 Numerical simulation of liquid flow in a rotating and partially filled cylindrical cavity, by *Sergio de Albuquerque Souza*

Coating fluid flows, which lead to the formation of a thin fluid film and are internal to the surface of the partially filled centrifuge cylinder, generate a great scholar/industrial interest,

since equipment based on this special type of flow can be used for a range of engineering applications such as coating, drying, cooling (melting) and evaporation/boiling. To obtain faster results and with reduced costs, several studies are used to model as well as to simulate processes in engineering. For the simulation presented, the OpenFOAM CFD tool is used for flow simulations involving two incompressible and isothermal immiscible fluids using a phase-to-phase capture approach based on VOF volume fraction, optional computational mesh movement and mesh topology changes including adaptive re-mesh. Due to the advantages offered by the OpenFOAM software, such as the possibility of using complex geometries, unstructured meshes, multigrid techniques and parallelization of data processing, besides being a free and open-source software, the numerical simulation of the flow of a liquid in a partially filled cylindrical cavity turn to be very dynamic and adapted to the problem.

CHT-21-186 Laminar flow heat transfer through a square duct with combined transverse ribs and helical screw tape inserts, by *Hrishiraj Ranjan and Sujoy Kumar Saha*

The thermo-hydraulic characteristics of transverse rib and full-length screw tape inserts in the square duct for five different fluids, are investigated and reported in this paper. The numerical investigations have been validated with the experimental published results and the variation in results are less than 18 percent. The numerical investigation was done with five different fluids: air, water, ethylene glycol, Servotherm oil and liquid sodium. The combined configuration for numerical investigation having transverse ribs and helical screw tape inserts were developed with design modeler module. The grid independence test was performed and the uniform sized grid was imposed on the geometry. The grid independence test suggested that 0.4 mm size of elements are good enough. The results of grid independence test are presented in the paper. For the numerical analysis, The ANSYS Fluent 19.2 was used. First, the physical problem was translated into mathematical form. The equations and the boundary conditions were standard boundary layer N-S equations and energy equation in tandem with continuity equation, respectively. The convergence criteria for continuity equation are 10^{-5} , for x, y and z velocity components and energy equation as 10^{-8} and 10^{-7} respectively. The temperature profiles along the duct wall and along the periphery of the screw tape inserts are reported. The streamlines along the duct, temperature profile at different sections is shown in figures. The two dimensionless rib heights, two dimensionless rib pitch and three screw tape parameters are considered. The effect of rib height, rib pitch and screw tape parameters on Nusselt number and the product of friction factor and Reynolds number are presented in the paper. The increase in rib height and decrease in rib pitch, increase the Nusselt number and product of friction factor and Reynolds number. The increase in screw tape parameter, decreases the Nusselt number and the product of friction factor and Reynolds number. On increasing Reynolds number, the Nusselt number and the product of friction factor and Reynolds number, both increases.

CHT-21-188 Orthogonal array optimization of the operational parameters for air-cooled cylindrical lithium-ion battery module, by *Dinesh Kumar Sharma and Aneesh Prabhakar*

High energy density and the high specific power of Lithium-ion batteries (LiBs) make it an ideal candidate for energy storage in electric vehicles. LiBs are very sensitive to temperature, and therefore proper battery thermal management is required during its operation in order to

maintain the cell temperature within a narrow range of 15 to 35 °C. In this study, an orthogonal array optimization for airflow velocity, C-rate, and battery cell arrangement for air-cooled battery thermal management strategy is proposed. Results from an experimental study using 32 LG INR18650 MJ1 cylindrical battery cells has been used in the present study. The battery cells were arranged in a 4P8S combination to make a total power capacity of 0.52 kWh. The metrics used to the optimum thermal performance of the proposed thermal management strategy are (i) maximum temperature in the module, and (ii) the maximum temperature difference between battery cells. Higher airflow velocity decreases the maximum temperature, while higher C-rate increases the maximum temperature and temperature difference in the battery module. Optimum parameters setting was found as airflow velocity of 0.6 m/s at 1°C discharge rate for cross battery cell arrangement.

CHT-21-191 Numerical analysis of turbulent heat transfer in rectangular duct, by *Jan Kren, Blaz Mikuz and Iztok Tiselj*

Numerical simulations of heat transfer near 25µm thick heated steel foil that covers part of the duct wall have been made jointly with the experiment at the Jožef Stefan Institute to study temperature fluctuations at the fluid-solid boundary. Results in the present paper are obtained at Reynolds number 10000 in a square duct geometry. The flow and heat transfer in the new experiment have been reproduced with a wall-resolved Large Eddy Simulation (LES) using a wall-adapting local eddy-viscosity (WALE) model in OpenFOAM computer code. Specific numerical cases range from an ideal isoflux boundary condition, which could be theoretically achieved with infinitely thin heated foil, to the realistic boundary condition, where heat transfer in the thin metal foil with a layer of paint is calculated. Since the thermal boundary layer is very thin, the passive scalar approximation is sufficient for qualitative assessment. However, temperature dependent viscosity substantially improves the accuracy of the results. Moreover, the conjugate heat transfer turns out to be a vital improvement of the study for the accurate determination of the magnitude of temperature fluctuations.

CHT-21-195 Experimental and numerical study of the effect of composition on GaN thin films grown by deposition, by *Omar Dhannoon Jumaah and Yogesh Jaluria*

Gallium nitride (GaN) thin films provide an attractive material for manufacturing optoelectronic devices for various practical applications due to their wide band-gap and superb optoelectronic performance. The reliability and durability of the devices depend on the quality of the thin films. Metal-organic chemical vapor deposition (MOCVD) process is a common technique used to fabricate high-quality GaN thin films. The deposition rate and uniformity of thin films are manipulated by controlling operating conditions and reactor geometry configuration. In this study, the epitaxial growth of GaN thin films on sapphire (AL₂O₃) substrates is carried out in a vertical rotating disk MOCVD reactor. The surface morphology and crystal quality of GaN thin films have been examined using Atomic Force Microscopy (AFM) and Scanning Electron Microscope (SEM). The results show that the composition of the inflow gases that determine the flow rate of the precursor trimethylgallium (TMG) and the carrier gas has a significant effect on the deposition rate and uniformity of GaN thin films. A detailed numerical study is also carried out. The numerical results confirm the trends seen in the experiments. It also allows expanding the study to include a wider range of operating conditions and reactor designs. It is

seen that the process can be optimized to obtain high quality films at acceptable deposition rates.

CHT-21-196 Heat transfer enhancement in a two-phase immiscible flow in microchannel, *by V. C. Teixeira, A. G. B. da Cruz, G. M. Guerra and F. P. Duda*

In this study, the convective heat transfer enhancement in a microchannel with immiscible droplets into a continuous phase liquid flow is analyzed by performing a phase-field model consisting of the coupled Navier-Stokes/Cahn-Hilliard equations and energy equation. Using a co-flow device producing spherical droplets in a dripping regime and based on the local and average Nusselt number and the temperature field distribution, we discuss the significant heat exchange increase with the spherical droplet-laden flow, compared with the case of single-phase flow.

CHT-21-197 Extreme (stochastic/random) boiling in the cryogenic zone, *by Charles Janeke*

In order to beat M10 continuous-flow infrastructure, cryogenic means of boiling liquid air (CRYOGENIC KETTLE©) synthesis has been invented whereby the motive power driving blowdown and continuous flow wind-tunnels may be enumerated by a factor of 10^3 in the M10 domain. In order to beat nucleate stagnation associated with linear/Newtonian boiling the ((vortex)) transformation power of the HYPERSONIC STOCHASTIC SWITCH© (USP 9550586) is inversely applied to transform ROSENSHAW boiling into an enumerated GAUSS-MARKOV stochastic process in the cryogenic zone by ((complex)) transformation of the 1st moment (derivative) of randomness/ applied to the controlling ΔP and ΔT (root) variables.

CHT-21-198 Numerical study of natural convective heat transfer from a horizontal two-dimensional two-sided plate having either a central gap or an adiabatic center section, *by Santiago del Rio Oliveira and Patrick H. Oosthuizen*

A numerical study of natural convective heat transfer from a plane horizontal, two-dimensional, two-sided isothermal plate, i.e., there is heat transfer from both the upper and lower sides of the plate, has been undertaken. The plate either has a central adiabatic section or a central gap (hole) and the main purpose of the study was to determine the effect of the size of this adiabatic section or of the central gap on the heat transfer rate from the plate. The mean flow has been assumed steady and symmetrical about the center plane through the plate. The range of conditions considered include those under which turbulent flow could develop and the k-epsilon turbulent model with buoyancy force effects accounted for has been used in obtaining the solution. The numerical results have been obtained using the commercial CFD code Ansys-Fluent©. The mean heat transfer rates from the plate for the two cases, i.e., adiabatic central section, or central hole, have been expressed in terms of mean Nusselt numbers which depend on the value of the Rayleigh number, on the dimensionless distance between the heated portions of the plate, and on the Prandtl number. Attention has been restricted to the case where the heat transfer is to air and the Prandtl number has therefore been assumed to be constant. Extensive investigations of the effect of the

dimensionless gap between the heated sections of the plate on the variation of the Nusselt number with Rayleigh number has been undertaken for the two cases considered.

CHT-21-199 Thermo-economic analysis of S-CO₂ power cycles for waste heat recovery applications, by **Francisco M. Miller, Manuel E. C. Cruz and Marcelo J. Colaço**

Supercritical CO₂ (S-CO₂) power cycles for nuclear power or concentrated solar power applications have been simulated and optimized usually aiming maximum efficiency, in order to reduce cycle's heat input. On the other hand, S-CO₂ power cycles for waste heat recovery applications have been optimized aiming to maximize waste heat recovery and useful power. Nevertheless, they demand a large Waste Heat Recovery Unit (WHRU) for this purpose, which usually costs from 30% to 50% of total system cost. In this paper, a thermo-economic study of a waste heat recovery S-CO₂ power cycle coupling the WHRU was performed. It was found that the significant cost of the waste heat recovery unit may affect the economic feasibility of the system.

CHT-21-201 Electrochemical thermal modelling of Li-Ion battery cell at different discharge rates, by **Arundas Odungat and Samarjeet Chanda**

Li-ion batteries are widely used in energy storage systems (ESSs) due to their high energy density. Prolonged usage of Li-ion battery packs often results in elevated temperatures within the cells which give rise to safety concerns. Efficient thermal management of battery packs using Battery Thermal Management Systems (BTMS) is the key to mitigating safety issues. Different electro-chemical-thermal (ECT) models are available in the literature that can predict the heat generation in Li-ion batteries, a key input for the design of efficient BTMS. This work is focused on using NTGK (Newman, Tiedmann, Gu, and Kim) model for predicting the temperature and heat generation of a pouch type Li-ion cell when it is discharged at different C-rates. A naturally cooled pouch type Li(NiCoMn)O₂ cell is numerically simulated. Simulations are performed for constant ambient air temperatures and different but constant rates of discharge. The model predictions show that with increase of C-rate average surface temperature increases and higher temperature region is observed near to the tabs necessitating the development of efficient thermal management systems for battery packs.

CHT-21-203 The GeTe thermal conductivity, from experimental measurement to DFT simulation, by **Jean-Luc Battaglia, Kanka Gosh, Clément Chassain, Andrzej Kusiak, Pierre Noé and Helcio Orlando**

A new photothermal radiometry technique, based on periodic pulses waveform, has been developed to investigate the thermal conductivity of phase change chalcogenide materials (PCM) deposited as thin films on a silicon substrate. The thermal conductivity of the PCM is identified within a large temperature range from experimental data using first a nonlinear least squares technique that gives initial set of values for a Markov Chain Monte Carlo based technique. The parameters involved within the phonon scattering characteristic time models, regarding the Umklapp and defects scattering processes mainly, are then identified using the MCMC approach in order to explain the role of the crystalline state of the PCM at different

temperatures with respect to the measured thermal conductivity. Application will focus on the GeTe PCM alloy due to its application in the field of phase change memories.

CHT-21-206 A new method based on artificial neural network for radiative heat transfer calculation: Comparison with benchmark numerical solutions in homogeneous media, by **Alex Royer, Olivier Farges, Pascal Boulet and Daria Burot**

A new method based on predictive capacity of feedforward artificial neural networks (FANN) is proposed, to estimate the divergence of the radiative flux in an axisymmetric domain very efficiently. Training and validation databases have been built thanks to results given by the SNB-CK model and computed accordingly with Monte Carlo formulation. The major aim of this work is to combine advantages of spectral models in terms of accuracy and the computational efficiency of neural networks and obviously, make possible the precise modeling of radiative transfer on an industrial scale. We show that ANNs are able to model almost perfectly the radiative flux divergence under certain conditions on the basis of training data. We also give here some keys to avoid the pitfalls related to ANNs.

CHT-21-210 An inverse analysis of the brain cooling process in neonates using the particle filter method, by **Felipe S. Nunes, Helcio R. B. Orlando and Andrzej J. Nowak**

The goal of this work was to sequentially estimate the transient temperatures of the brain and other body regions, during systemic cooling of a neonate. The body was divided into spherical or cylindrical elements representing the head, thorax, abdomen, arms and legs. Each body element included multiple tissue layers and was further divided into two sectors to allow nonuniform heat transfer with the surrounding environment. Pennes' model was applied in each body element and Fiala's blood pool concept was used for the solution of the forward bioheat transfer problem. A state estimation problem was solved with the Sampling Importance Resampling (SIR) algorithm of the Particle Filter method. The results obtained with simulated temperature measurements revealed that the Particle Filter method was accurate for the estimation of the internal body temperatures. Therefore, such technique has great potential to perform as an observer of the brain temperature of neonates, for the analysis and control of the systemic cooling treatment of neonatal hypoxic-ischemic encephalopathy.

CHT-21-211 Improving efficiency of a micro-thermophotovoltaic power generator with various recuperator configurations, by **Seok-Beom Yun, Sung Yeon Kim and Youn-Jea Kim**

A micro-thermophotovoltaic (TPV) power generator uses a hydrogen-air mixture as fuel to convert chemical energy into radiant energy. Radiant energy flows to a photocell and charges it with electrical energy. Therefore, it is desirable that the wall temperature of the micro-TPV power generator remains high and uniform. In this study, the influence of the geometric dimensionality of the computational domain was analyzed by performing numerical simulations with three-dimensional grid systems. A poly-hexcore mesh type was applied to reduce errors caused by convection and diffusion. The model incorporates a heat recuperator to improve fuel efficiency and apply the blanket effect for better thermal performance. The

results are compared with experimental data from existing publications using computational fluid dynamics (CFD). In numerical analysis, the eddy dissipation concept (EDC) model for species transport was used to accurately calculate the interaction between the turbulence and chemical reactions. Sensitivity analysis of the independent variables of the geometrical configuration was conducted for the parameter study. The results of the modified model, which has a higher average wall temperature, are graphically analyzed and compared with a reference model using contours for the velocity, temperature, and effective Prandtl number.

CHT-21-212 Influence of dimpled-wall tubes on the thermal performance of the plate-fin-tube heat exchanger, by **Sung Yeon Kim, Seok-Beom Yun** and Youn-Jea Kim

Plate fin-and-tube heat exchangers are used in various industries. Recently, many studies have been conducted to improve the performance of the plate-fin tube heat exchanger using computational fluid dynamics(CFD). Various studies of fin configurations have been proposed to enhance thermal efficiency but relatively few studies of tube configurations are conducted. In this paper, the effects of dimpled-wall tubes on the flow characteristics and the thermal performance of the heat exchanger are studied using numerical analysis. In particular, the operating condition($Re = 360$) is considered to compare dimpled-wall features with the reference model which has no dimple. To evaluate the performance of the heat exchanger, characteristics of heat transfer and pressure drop are analyzed using velocity field, Colburn factors, Fanning factors, and the area goodness factor. Overall, tubes with dimpled-wall showed a greater performance of area goodness factor considering the relationship between the heat transfer and the pressure drop. The largest heat transfer performance occurs at the dimple shape ratio of 0.18 of 11.7% improvement over the reference model.

CHT-21-214 Study of radiative heat transfer in nucleate boiling under microgravity conditions, by **M. Naarendharan** and Ankit Bansa

Nucleate pool boiling has widespread applications in microgravity environments ranging from thermal management, storage of cryogenic propellants to electronic cooling required in satellites. In this research, a numerical study is carried out to realize the effect of radiation heat transfer in pool boiling - single bubble under microgravity conditions. The effect of radiative heat transfer becomes increasingly significant at low gravity conditions due to low buoyancy resulting in the diminishing effect of natural convection. The solver "evapVOFHardt" based on the Volume of Fluid method available in Open source software - OpenFOAM was used and modified to include radiative heat transfer to analyze the current research. The solver was validated with data from the literature. It is found that the departure diameter varied with gravity as $g^{-0.5}$ while the departure time followed a trend of $g^{-0.93}$. Phase change happens at the interface between the vapor and liquid phase, with the superheated layer around the interface augmenting the phase change. At zero gravity conditions, due to less buoyancy, the departure diameter and the departure time of the bubble from the base increase drastically from that at normal gravity conditions. Due to the bubble's longer stay at the base, radiative heat loss from this superheated layer causes less amount of heat to go into the evaporation of the liquid. Thus, an increase in the departure time and can eventually alter the departure diameter of the bubble. This study utilizes the fvDOM and P1 methods to solve the radiative transfer equation and deduce radiation's effect in boiling at microgravity. It was

observed that the departure time and the departure radius of the bubble had an average increase of 2.87 % and 0.56 %, respectively at lower gravities such as 0.05g and 0.03g. Although the radiation is insignificant at these gravity levels, one may expect significant effects at much lower gravities like $10^{-4}g$ and for higher saturation temperatures of the working fluid.

CHT-21-217 Large eddy simulation of jet -impingement on flat plate using sub-grid scale models, by **Ashutosh Narayan Singh and Dushyant Singh**

In the present study, a slot jet impingement of air over an Isothermally heated plates cooled by incompressible and turbulent jet is numerically analyzed by Large-Eddy Simulation (LES) at the nozzle to plate spacing, $h/2S = 3.5$, Reynolds number 22,500 for heat transfer and 23,400 for fluid flow cases, Using three SGS (sub-grid-scale) models ie WALE(Wall-Adapting Local Eddy-viscosity), dynamic k-equation models and Smagorinski model. Numerically using Open Foam, an open-source finite-volume based CFD code. Spatial and temporal averaging of velocity is performed to give information of fluctuating velocity variances ie Reynolds Stress. Different significant dynamical stream structures have been envisioned from the instantaneous computed data solver. The local Nusselt number results, near-wall fluctuating velocity variances were in good resemblance with experimental results of Narayanan et . al. WALE and Dynamic k equation model were in good agreement with experimental results.

CHT-21-219 Molecular dynamics study on interactions between wall surface and solidification interface of water molecules, by **Uchida Shota, Kunio Fujiwara and Masahiko Shibahara**

In this study, we investigated interaction phenomena between a solidification interface of water and silanol-terminated silica surface, by conducting the non-equilibrium molecular dynamics simulations. We investigated the effects of the interaction strengths between water molecules and the silica surface on the density profile of water molecules in the vicinity of the silica surface, when the solidification interface contacted the silica surface. The results revealed that when the interaction strength between water molecules and silica surface were relatively weak, water molecules crystalized on the silica surface and the density distribution of water molecules in the vicinity of the silica surface depended on the ice crystal state. On the other hand, in the case of the strong interaction between water molecules and silica surface, the ice crystals were not formed on the silica surface when the solidification interface contacted the silica surface.

CHT-21-220 State estimation problem in nano-enhanced phase change materials for thermal energy storage, by **Bruno dos Reis Jaccoud, Helcio Orlande, Marcelo Colaço, Ryszard Bialecki, Zbigniew Buliński and Ziemowit Ostrowski**

Phase change materials (PCM) have become increasingly important in the last few years for the thermal storage of renewable energy. This work deals with the numerical simulation of a PCM containing metallic nanoparticles, used for the thermal storage of solar energy. Energy, momentum and mass conservation equations were solved numerically using finite volumes together with the enthalpy method, for a two-dimensional rectangular geometry, taking into

account buoyancy effects. Paraffin ($C_{28}H_{58}$) was adopted as the phase change material, containing copper nanoparticles with 1% volume concentration. The Particle Filter method was applied to estimate the energy stored in the phase change material under direct solar irradiance from non-intrusive temperature measurements, by solving a state estimation problem. In order to reduce the computational cost associated with the solution of the state estimation problem, a reduced model was used, based on the Proper Orthogonal Decomposition technique with Radial Basis Functions. The coefficients for the POD basis were expressed as a linear combination of radial basis functions, for the variables of interest. Results obtained with simulated measurements revealed the accuracy of the proposed technique for non-intrusive indirect monitoring of the energy stored in the phase change material.

CHT-21-223 Modeling and identification of mathematical model of high-temperature superconducting coil, by *Oleg M. Alifanov, **Aleksey V. Nenarokomov**, **Aleksey G. Vikulov**, Alena V. Morzhukhina, Sergey A. Budnik and Vladislav V. Ilyin*

The two-model iteration method is applied to plan a test for getting temperature distribution in time as additional information completing formulation of identification problem. In this work we just apply first approach of the thermophysical properties putting them into a detailed model of prototype. It is used then to calculate experimental regimes and identify an intermediate model in the scope of the method which basics are cited briefly. The variation iteration method is applied to regularize unstable solution for not contractive mapping when an iteration process does not converge according to the Riesz theorem. Finally, temperature fields calculated on the detailed model are shown dependent on the time and space coordinates. Properties of the intermediate model identified on those temperatures are dependent on temperature as given temperature is a function from time.

CHT-21-224 Influence of a flexible vortex generator on hydrodynamic and heat transfer characteristics of a pin-fin array, by ***Seyedmohsen Baghaei Oskouei** and Özgür Bayer*

Flexible vortex generators have recently gained attention in terms of their hydraulic and thermal effects in different applications. In the present study, a singular vortex generator as a flexible beam attached to a pin-fin is considered in an array of staggered pin-fins. A 2D model is developed from an already available microchannel heat-sink design that uses 15 cylindrical pin-fins in a staggered configuration from the literature. The laminar flow is coupled with the elastic solid domain. To solve the fluid-solid interaction equations, the arbitrary Lagrangian-Eulerian methodology is employed using a commercial software that utilizes Finite-element method. The numerical model is validated with respect to two procedures to ensure the safety of the method. The effect of moving vortex generator in the vicinity of the pin-fins is studied and the movement of the generated vortex at the tip of the beam through the flow and its effects on the main flow are investigated. A simple energy balance is at work to study the thermal performance of the design. In terms of pressure drop, an enhancement of near 4% is observed while the overall thermal efficiency of the system is found to be 3.6% improved compared to the heat-sink without vortex generator.

CHT-21-225 A computational study on hydrous ethanol flame development in a spark ignition engine, by **Fabiano Alves dos Santos** and **Albino José Kalab Leiroz**

A multidimensional computational model was developed using a commercial software to simulate the operation of a 1.4-liter flex-fuel engine cylinder fueled with hydrous ethanol. The Large Eddy Simulation (LES) model was used to describe the turbulent flow field. A detailed chemical kinetics mechanism with 380 species and 1194 reactions is used to describe the hydrous ethanol combustion reactions. The consistency of multidimensional numerical results was verified through the GCI method. The full load engine operating point at 3875 rpm and fixed stoichiometric ratio (with $\lambda=0.9$) was analyzed. The obtained results allow the observation of the velocity, temperature and composition in-cylinder fields throughout the engine operation four strokes. In the present work, the fuel-air mixture ignition, flame propagation processes and the regions within which NO_x producing reactions occur deserved particular attention. Turbulent flame speed values of 6.6 m/s (10% to 90% MBF) were obtained for hydrous ethanol within the engine in full load conditions. The wall heat flux, the mean in-cylinder pressure and temperature values are obtained from local numerical results and compared to experimental data for validation purposes. The shape and development of the flame were also analyzed. Results show that the combustion chamber geometry has a major influence on the flame characteristics. Departing from a spherical shape, the flame becomes stretched and displays cold and hot spots that could be precursors of knocking, and locus of NO_x formation and unburned gases.

CHT-21-226 Effect of various deposition configurations on film cooling characteristics of laidback fan shape hole, by **Ashutosh Kumar Singh**, **Dushyant Singh** and **Niranjan Sahoo**

The numerical study is carried out to understand the effect of various deposition configuration over the film cooling characteristics of the laidback fan-shaped hole. The present study is carried out for the fixed blowing ratio (M) = 1, density ratio (DR) = 2.42 and mainstream Reynolds number (Re_{ms}) = 4000, and secondary stream injection angle of 35°. The work presents here is focused on the deposition location and deposition height. Three different deposition locations are placed over the flat surfaces. The centerline and lateral average effectiveness of with and without depositions are compared for various locations and deposition heights. The study reveals that film cooling characteristics of the shaped hole are significantly affected by the variations in deposition location and deposition heights. With the increase of deposition height from h/D (0.3 to 0.7) lateral average effectiveness reduces downstream of deposition locations. Moreover, the increase in the deposition locations from the downstream of hole directions improves film cooling effectiveness upstream of deposition location.

CHT-21-227 Optical properties and thermal conductivity of heat-insulating material based on mesoporous silica with various thermal radiation absorbers, by **Roman A. Mironov**, **Olga V. Tomchani**, **Viktoria O. Guydenko** and **Maxim O. Zabezhailov**

Thermal insulation material composed of fiber-reinforced mesoporous silica with and without the addition of silicon carbide, titania and zirconia opacifier was produced and characterized. Optical properties (scattering and absorption coefficients) were experimentally determined

in the spectral range of 0.9 – 4.7 μm by inverse problem of radiative transfer solution. The inverse problem relied on invariant embedding equation and measured spectral directional-hemispherical reflectivities. The effect of silicon carbide opacifier addition on the optical properties and Rosseland mean radiative thermal conductivity was estimated. Calculated radiative thermal conductivity of thermal insulations with various volume fractions of SiC opacifier was compared to the radiative thermal conductivity deduced from the effective one, which, in its turn, was measured by quasi-stationary technique with a self-made setup. The results of the inverse problem solution were compared to the calculations based on Mie theory and measured silicon carbide particle size distribution. The size distribution of SiC opacifier was numerically optimized to obtain as low as possible Rosseland mean radiative thermal conductivity. Radiative thermal conductivities of thermal insulations opacified with various zirconia and titania powders were estimated using Mie theory and Rosseland approximation on the base of experimentally measured powders size distributions. Theoretical predictions were compared to the experimentally determined effective thermal conductivity. Finally, the effect of Fe_2O_3 , Si_3N_4 , TiO_2 , graphite, ZrO_2 , TiN, TiC, AlN opacifiers was analyzed numerically using Mie theory. Titanium-based compounds and iron sesquioxide were shown to be perspective opacifiers for high temperature applications.

CHT-21-228 A particle-filter based framework for inverse problems using ANSYS Fluent and Python, by **Bruno Henrique Marques Margotto, Carlos Eduardo Polatschek Kopperschmidt, Marcelo José Colaço, Wellington Betencurte da Silva, Julio Cesar Sampaio Dutra and Luiz A. S. Abreu**

It is quite common to most thermal engineering problems the lack of information relating to the boundary conditions, due to technical or economic limitations. For this reason, inverse heat transfer problems techniques have been developed to overcome such problem. The general interest lies in parameter and state estimation for unknown and desired properties. To accomplish that, it is required to solve a direct problem of the thermal phenomena, which are described by differential equations. In many applications, such solution is determined by numerical methods, such as the Finite Volume Method (FVM). In this regard, ANSYS Fluent is a FVM-based software which solve differential equations with relative simplicity considering its friendly and easy interface. Once the direct problem is defined, a Bayesian Filter can be applied for the inverse problem. Due to robustness, the Bayesian Filter named Particle Filter (PF) is widely applied to state and parameter estimation. In this work, we aim at the application of SIR and ASIR Particle Filters to estimate the values of parameter and state of a transient microheat exchanger. The methodology also considered sequential use the softwares ANSYS Fluent and Python respectively for the direct problem (FVM) and inverse problem (PF). Three different inlet velocity profiles were studied: constant, step and ramp-like changes. The results show satisfactory estimation, which allow concluding that the developed tool seems promising to more complex geometries and physical model problems.

CHT-21-229 Systems based CFD modelling of package steam boilers, by **Peter Klein, Marinus Potgieter and Bianca Ferreira**

Dynamic thermo-fluid models of fire-tube steam boilers can be used to optimise the design and operation of equipment, resulting in possible energy and emissions savings. This work presents the development of a dynamic boiler model of a 4-pass wetback fire-tube boiler,

using the commercial 1-dimensional CFD tool Flownex®. The thermal model includes all relevant heat transfer and fluid flow phenomenon between the combustion flue gasses and the boiler water/steam. The predicted exhaust flue gas temperatures at different operating pressures are compared favorably to the performance data for a PFTA500-4 boiler, with accuracy improvements over previous modelling studies in the literature. Finally, the transient simulation capabilities of the model are demonstrated for a case of varying steam demand levels, with PID control algorithms implemented to control the feedwater control valve on the mass flowrate of fuel to the boiler. The modelled control system will be further refined in future work to include oxygen trim control over the air/fuel ratio. The completed model will be integrated into larger steam generation and distribution steam networks in Flownex, to assist industrial companies in South Africa in improving their energy efficiency.

CHT-21-230 Solar hybridization paths for cement production processes, *by Ilker Tari and Onur Polat*

Cement industry is responsible for a significant portion of global carbon dioxide emissions leading to global warming and climate change. A substantial part of these emissions is due to burning fossil fuels to supply heat to the kiln at a high temperature. Concentrating solar collectors can be used for preheating the air supplied to the kiln or for directly preheating the ingredients in the pre calciner before feeding them into the kiln. Based on an existing cement plant's available energy audit, a Matlab model of the plant with its sub-processes has been developed. After validating the model by checking the model results against the energy audit's mass and energy balances, the model is used to identify the possible solar hybridization paths. Considering the year-round solar resources in the region where the plant is located, it is shown that there are hybridization paths leading to significant carbon dioxide emission savings.

CHT-21-232 CHT modeling of an electronics cabinet using multi-scale meshing, *by Ilker Tari and Yanki Cobanoglu*

An electronics cabinet populated with various components, including two workstations, an uninterrupted power supply, and networking equipment, is experimentally and numerically investigated. Experimental temperature measurements were taken on different locations surrounding the components using type-K thermocouples and a data logger for 8 hours in which the cabinet was in steady-state. These measurements were then used to validate the numerical model created in commercially available computational fluid dynamics software ANSYS Icepak. First, the model for Workstation-1, one of the significant components inside the cabinet, is presented since most of the information on its thermal behavior is available. Mesh independence analysis was done, and the conservation of mass and energy was checked. Next, the whole cabinet was modeled, consisting of other components and the rack-frame within a domain of average room size. Steady-state Navier-Stokes equations were solved along with $k-\epsilon$ turbulence equations with variable material properties to account for natural convection effects. A multi-scale mesh structure at different mesh densities for inside the components, the cabinet, and the room is formed for analyzing the entire cooling solution, including the heat rejection to the walls of the room. A grid-independent solution is obtained and validated using experimental measurements. The validated model was used for investigating different front cover patterns with various opening ratios and solutions to prevent limit excess. Results show that blanking panels are viable solutions to prevent

leakages. The 85%-open front cover can be used, whereas 25% one cannot be. A variable-free-area-ratio cover that was designed based on limiting the segmental flow leakage results from the simulations is suggested and tested. It was observed that it could be an effective solution if used together with a blanking panel preventing leakage from the power distribution unit outlet.

CHT-21-235 RANS based numerical simulations of turbulent diffusion flame using OpenFOAM®, by **Amit Makhija and Krishna Sessa Giri**

The present work showcases simulation of a turbulent diffusion flame for validation of the turbulence-chemistry interaction approach. The turbulence model employed was $k-\epsilon$ with the model constants determined from simulation of a non-reacting turbulent jet. The jet decay rate and spread rate were determined with excellent accuracy when compared with experimental measurements. The non-dimensional velocity profiles also show a significant agreement except at radial locations far away from the axial centreline. Simulations of the DLR-A flame using a single step infinite rate chemistry assumption were carried out with the model constants thus determined. The reaction rates are determined based on the mixed-is-combusted approach where the mixture fraction, a conserved scalar quantity is obtained by the solution of a governing equation. In addition the mean velocity, species mass fractions and temperature profiles in the axial and radial direction are compared with experimental data. The axial profiles show very good agreement while the radial profiles show deviations due to the assumption of equal binary mass diffusivities for all species and unity Lewis number, which is a suitable approximation for turbulent gaseous flows. In addition, the temperatures are overpredicted by close to 15% due to the single-step infinite rate chemistry approach adopted in this study. The validation serves to justify the choice of the combustion model for the simulation of turbulent reacting flows. This is especially significant due to the lesser computational effort involved in obtaining the rates of the reaction for a turbulent diffusion flame.

CHT-21-240 Numerical study of latent heat thermal energy storage based on an innovative hexagonal heat exchanger: Performance evaluation, by **Imad Ait Laasri, Zakaria Elmaazouzi, Abdelkader Outzourhit, Mustapha El Alami and El Ghali Bennouna**

Thermal energy storage (TES) is a major challenge for the development and implementation of concentrated solar power (CSP) plants. Recently, latent heat thermal energy storage (LHTES) has gained the most interest in research because it has the advantage of increasing the energy density through the use of phase change materials (PCM). However, the main limitation of PCMs is the low thermal conductivity, which has a poor effect on the system performance. For this reason, several designs of heat exchangers have been proposed to overcome the decrease in the heat transfer rate. For this purpose, this numerical study will analyze the charging and the discharging behaviour of a new honeycomb structure never used in LHTES cylindrical systems, which is examined using the simulation software « COMSOL Multiphysics » that is based on the finite element method. The system includes NaOH-NaNO₃ as the phase change material (PCM), with DelcoTerm Solar E 15 as heat transfer fluid (HTF). The main objective of this study is to evaluate the performance of a new innovative hexagonal heat exchanger (honeycomb finned structure) and to compare it with a coaxial heat exchanger without fins.

The results presented show a maximum increase in performance of 66.88% and 58.04% during charging and discharging processes respectively, with the use of temperature contour maps, temperature curves, melt fraction and state of charge plots as a function of time to evaluate the heat transfer characteristics of this innovative LHTES unit.

CHT-21-242 Sequential boundary heat flux estimation using the method of Fundamental Solutions and Bayesian filters, by **Carlos Eduardo Polatschek Kopperschmidt, Bruno Henrique Marques Margotto, Carlos Eduardo Rambalducci Dalla, Marcelo Jose Colaço, Wellington Betencurte da Silva and Julio C. Sampaio Dutra**

In many thermal engineering problems the boundary conditions are not fully known, since there are technical difficulties in obtaining data. When boundary data is inaccessible, for example, it is necessary to deal with an Inverse framework to reach this unknown information. To obtain the solution of an inverse problem as an iterative process the direct problem needs to be called repeatedly which makes meshless methods implementing, as the Method of Fundamental Solutions (MFS), attractive. In the MFS procedure a linear system of fundamental solutions is solved in order to obtain the solution of the respective partial differential equation (PDE) from the studied problem. To solve the parabolic heat equation without needing to perform transformation of the Parabolic equation into Elliptic or treat the time component separately the fundamental solution of the parabolic heat equation was used. The presented case consists in a classical one-dimensional IHCP of boundary heat flux estimation using intrusive measurements. The inverse problem was solved by three different Bayesian filters schemes combined with the MFS: Sampling Importance Resampling (SIR) filter, Auxiliary Sampling Importance Resampling (ASIR) filter and Unscented Kalman Filter (UKF). The measurements from the inverse procedure were generated using Finite Difference Method (FDM) to avoid the inverse crime. The presented results shown good agreement in the three schemes even using few collocation points in the MFS procedure.

CHT-21-244 Influence of particle shape on turbulence induced flow dynamics and heat transfer in packed beds, by **Mona Al-Mqbas, Nico Jurtz and Matthias Kraume**

The dynamics of turbulent structures in flows within the packed beds are of special interest for chemical processes. These structures play a critical role in the transport of mass, heat, and momentum within randomly packed beds. The inertial terms in these turbulent flows strongly modify the flow field leading to the appearance of vortices and jets within the pore-region between the bed particles. Such flow patterns contribute to the dispersion of chemical species and the transfer of heat and mass. Although, with the help of computation fluid dynamics, transport processes in packed bed reactors have been studied intensively in the last years, only little attention was given to the fundamentals of turbulent effects. The influence of the global geometrical characteristics of the bed particles on the turbulent heat transfer remains unknown. In the present study, Large Eddy Simulations are performed on a volume extracted from a randomly packed bed to study the influence of particle geometry on the flow. The complexity of the particle surface configuration is increasing from a circular to a multi-lobe and grooved cylinder. The influence of the surface smoothness on the turbulent flow and heat transfer is going to be quantified. The flow topology and the turbulence quantities like mean

and root mean square values (velocity and temperature), covariance of velocity, turbulent heat flux, and Kinetic energy transport and its dissipation rate will be analyzed.

CHT-21-249 Dynamic GMAW process model for layer geometry control in wire arc additive manufacturing, by **Rafael M. Bendia**, **Fernando Lizarralde**, **Augusto V. Passos** and **Victor H.P.M. Oliveira**

Wire Arc Additive Manufacturing (WAAM) is a large-scale metal AM technology that uses an electric arc to melt a metallic filler wire in order to produce near net-shape metal parts by depositing layers of molten metal on top of each other. The accuracy of the layer geometry during deposition leads to decreased material consumption and post processing machining costs, as well as reducing the occurrence of internal voids in the produced part. Closed-loop control can be used to guarantee a more precise deposition geometry. Thus, the relationship between the deposition parameters and the layer geometry (layer height and wall width) needs to be established in order to control the WAAM process. This paper focuses on modelling this complex mass and heat transfer problem for control design. It proposes a static model for predicting the deposited layer geometry of thin walls using process variables (wire feed speed, travel speed and contact tip to workpiece distance) and physical variables (arc power, inter-pass temperature) as inputs. The model is based on the well known Rosenthal solution for the temperature distribution due to a moving heat source in combination with a geometric parameterization of layer geometry. This layer geometry model is incorporated in a dynamic model of the GMAW process for control design and simulation. The proposed model is compared to experimental data produced by a GMAW power source using carbon steel filler wire for model parameter identification. Finally, PID controllers are proposed for the regulation of both layer height and wall width. Numerical simulation results illustrate the efficacy of the proposed control methods.

CHT-21-250 Transfer function estimation with SMC method for combined heat transfer: insensitivity to detail refinement of complex geometries, by **L. Penazzi**, **S. Blanco**, **C. Caliot**, **C. Coustet**, **M. El Haji**, **R. Fournier**, **J. Gautrais** and **M. Sans**

The optimization of thermal transfers in engineering systems such as heat exchangers requires the analysis of the influence of heat sources upon the temperature at various positions of interest in the studied system. In order to achieve the resolution of the combined modes of heat transfer through these systems, their couplings and the complex 3D geometries involved need to be integrated with full accuracy. Recent developments in probabilistic formulations in the context of transient combined heat transfer (linearized conduction-radiation-convection) have opened a new route to solving such problems with Monte Carlo (MC) algorithms, using state-of-the-art computer graphics digital libraries to handle complex geometries. To estimate the temperature at a probe point of interest, random paths are generated from its position and propagated through the geometry until a known temperature is reached. From a single MC calculation to sample the path statistics, the Symbolic Monte Carlo (SMC) method is used to express the probe temperature as a linear function of the sources. This function can then be used to estimate the probe temperature for any source values, alleviating the need to repeat Monte-Carlo simulations for each source condition, resulting in greatly reduced computation time. This approach is applied to the case of an open-

cavity porous medium and computation time insensitivity to the complexity and fineness of the geometry is demonstrated.

CHT-21-251 Numerical investigation of cavitating flow in a horizontal converging-diverging nozzle, by **Mohammed Zamoum, Rachid Boucetta and Mohand Kessal**

The objective of this paper is to investigate the dynamic evolution of cavitating flow in a horizontal converging-diverging Venturi nozzle. A nonlinear continuum bubbly mixture model coupled with the dynamics equation of the bubble is used to investigate the effects of the throat dimension of converging-diverging nozzle. Equation set is numerically resolved by the use of a fourth order Runge-Kutta scheme. The numerical resolution of the previous equations set let us found that the bubble radius distribution, fluid velocity and fluid pressure change dramatically with the throat length of the Venturi and an instability appeared just after the passing the converging nozzle for an throat length greater than 4.2 cm which correspond to the critical bubble radius $R_c = 6.85$. Also, we found that, the throat dimension of converging diverging nozzle has strongly affected the bubble frequency and the characteristics of the flow.

CHT-21-254 Modeling of conjugate heat transfer within thermal barrier coatings for combustion environments, by **Nicolas Tricard and Xinyu Zhao**

The inclusion of radiation modeling alongside conduction and convection has been a challenge in computational heat transfer. A 3D conjugate heat transfer (CHT) solver has been developed which integrates these three modes, targeting thermal barrier coatings within gas turbine combustors. The radiative transfer equation solver features an accelerated Monte-Carlo ray tracing method for structured orthogonal hexahedral meshes. The algorithm is analytically verified in a gray plane-parallel 1D medium with various configurations, including wall emission and isotropic scattering. The conduction and convection components account for the heat transfer from the interior flame to the TBC and the heat transfer to the exterior impingement flow from the adjacent alloy. The three-dimensional CHT code is further verified by comparing the results to those of a well-established one-dimensional CHT method for TBCs. This code is then tested in three dimensions using a non-uniform incident heat flux from the flame. Parametric variations of the heat flux distribution, material properties, and geometry are conducted to understand the relative importance of all modes of heat transfer.

CHT-21-255 AI-Machine learning algorithms for the simulation of combustion thermal analysis, by **Arunim Bhattacharya and Pradip Majumdar**

With the advances in big-data science and availability of current and emerging high-end computing powers such as the GPUs and cloud computing infrastructures, AI-Machine Learning (ML)/Deep learning (DL) methods are increasingly being used for predictive analysis and design analysis of variety complex engineering problems. ML/DL models are developed for various classes of problems involving large non-linear parameters from energy usage pattern in power distributions including renewable power sources; building energy consumption and management to improve energy consumption and efficiency to optimized

design and predictive analysis of thermal heat management systems in electronics and Li-ion battery storage systems. Objective of this paper is to explore the development of an AI/Machine Learning model for studying performance for predictive and design analysis of an internal combustion engine as an alternative to high fidelity computation fluid dynamic model. Machine Learning (ML)-Artificial Neural Network (ANN) algorithm is considered for characterizing and predicting the combustion process through use of historical performance data produced by computational model involving complex Multiphysics flow dynamics, heat transfer and chemical kinetics. Number of key ANN parameters such as number of hidden layers, number of neurons and activation functions are numerically experimented to achieve acceptable level of prediction accuracy through minimizing the training and validation losses.

CHT-21-257 Overheating in compressible heat transfer near the thermodynamic critical point due to non-normality, *by Luiz Ricardo C. de Almeida and Leonardo S. de B. Alves*

A thermodynamic model for the heat transfer taking place inside a cavity under microgravity is analyzed when one of the walls is suddenly heated to a constant temperature whereas the opposite wall loses heat by convection to the outside. This cavity contains a fluid whose thermodynamic state is slightly above its critical point, leading to the presence of strong compressibility effects. This problem is governed by two main control parameters, the gamma and Biot numbers. The former is the ratio between heat capacities at constant pressure and volume whereas the later represents the ratio between convection away from the surface and conduction inside the body. The temperature inside the cavity is obtained using spectral methods. Its mean value does not increase towards its steady-state monotonically. For gamma values higher than approximately ten and Biot numbers of order one, this mean temperature quickly increases beyond its steady-state and then slowly decreases towards it. In order to explain this behavior, an improved lumped analysis is performed to generate a simplified model for the mean temperature. Its eigenvalues reveal a stationary and stable behavior and, hence, cannot explain this temporary overheating. On the other hand, an analysis of its eigenvectors reveal a loss of orthogonality consistent with non-normal behavior that explains the temporary mean temperature increase above its steady-state. A direct numerical simulation of the compressible Navier-Stokes equations for the same problem confirms the existence of this overheating. Such a discovery can have important implications to heat transfer processes that employ supercritical fluids.

CHT-21-262 Computer-generated images of the absorption/scattering of a laser sheet in an heterogeneous medium by a new optimized Monte-Carlo method, *by Morgan Sans, Mouna El Hafji, Vincent Eymet, Vincent Forest, Richard Fournier and Najda Villefranque*

In combustion, the study of the influence of soot particles on radiative transfer as well as their characterization is commonly carried out experimentally through the propagation of a laser source in the visible range. Numerical simulation of diagnostic methods based on laser propagation helps to verify commonly formulated assumptions, provides useful support for identifying the sensitivity of parameters and highlights possible experimental constraints. In this paper, a numerical simulation tool based on a new reverse null-collision Monte-Carlo algorithm and used to produce computer-generated images resulting from the static scattering of light of a laser sheet by a heterogeneous absorbing/scattering medium is

developed. Such tool is applied to the study of a sooting medium described by the RDG-FA theory. Results highlight the influence of the main soot morphology parameters on the collecting signal.

CHT-21-266 Inverse heat transfer problem for the characterization of a palladium nanofluid, by **Nilton P. Silva**, *Cláudia C. R. Cruz, Henrique M. Fonseca, Leonardo A. B. Varon, Claudio L. Cesar, Dilson S. Dos Santos and Helcio R. B. Orlande*

Palladium nanoparticles can be used in the hyperthermia treatment of cancer due to their photothermal effects and biocompatibility. The aim of this work was to characterize a distilled water-based palladium nanofluid in terms of its physical properties. Specific heat was measured with Differential Scanning Calorimetry (DSC), thermal conductivity with the Modified Transient Plane Source (MTPS) method and dynamic viscosity with a rotational viscometer. A sample of the nanofluid was also pipetted into one well of a 96-well plate and heated by a diode-laser. Non-intrusive measurements of the local temperature at the top surface of the nanofluid were taken with an infrared camera during heating. A Bayesian approach was then applied to estimate the absorption coefficient of the nanofluid. Prior information available for model parameters was used together with the transient temperature measurements in the Markov Chain Monte Carlo (MCMC) method, implemented with the Metropolis-Hastings algorithm.

CHT-21-270 Viscoelastic fluid and Dean flow effects on flow and heat transfer characteristics of serpentine channel, by **Kazuya Tatsumi**, *Yousuke Tanaka, Reiko Kuriyama and Kazuyoshi Nakabe*

Viscoelastic fluid can increase the heat transfer coefficient of the low Reynolds number flow in the serpentine channel by generating unsteady and secondary flows. A pair of longitudinal vortices which is similar in form to Dean vortices is generated mainly due to the first normal stress differences. These vortices carry the low temperature fluid toward the channel sidewalls and increase the heat transfer coefficient. However, each contribution of the viscoelastic effect and the centrifugal force (Dean vortices) on the secondary flow and heat transfer characteristics are not clearly investigated and distinguished, especially in the case of serpentine channel. In this study, we conducted three-dimensional numerical computation on viscoelastic fluid in serpentine channel using Oldroyd model. The effects of the Reynolds number (Dean number) and Weissenberg number on the flow structure and heat transfer coefficients were evaluated. In the results, the viscoelastic flow and Dean flow gave certain similar aspects. However, the viscoelastic fluid generated stronger secondary flows and producing higher heat transfer coefficient for high Weissenberg number conditions. Further, we showed that the first normal stress difference plays an important role to characterize the flow, and good agreement can be obtained between the measurement and computation by introducing the dimensionless normal stress difference.

CHT-21-271 Heat transfer performance of a supercritical CO₂ based microchannels recuperator including thermal buoyancy, by *Janhavi Chitale and George S. Dulikravich*

Supercritical CO₂ (sCO₂) is used as a coolant for a wide range of applications from nuclear reactors to rockets and military aircrafts. One such application is compact microchannel recuperators used in Bryton cycle-based power plants, operating between 854 K at 9 MPa and 450 K at 22 MPa. Very few studies analyze effect of thermal buoyancy on the heat transfer during vertical flow of sCO₂ through microchannels. The current computational study analyzes the effect of flow acceleration on the buoyancy force and its relation to heat transfer performance of the recuperators. Mass flow rate corresponding to the target Reynolds number of 20,000 was applied at the hot and cold tube inlets to test the effect of turbulent flow regime on buoyancy force and in turn on the convective heat transfer. The effect of change in flow direction with respect to axial gravitational force was also studied. The conclusion is that the thermal buoyancy does not influence forced convection heat transfer in compact heat exchangers utilizing sCO₂ for the tubes with total length to hydraulic diameter ratio of thirty.

CHT-21-273 Numerical comparison of three different pin fin heat sink orientations, by *Eyub Canli, Mukaddes Ozdemir and Ahmet Ali Sertkaya*

Computational Fluid Dynamics (CFD) was used in order to simulate laminar natural convection heat transfer from a pin fin heat sink at three different orientations. Pin fin heat sink had 64 units of circular cross section pins. Pins were arranged in inline array. Constant spacing amount that is 14 mm between pins and 30 mm pin height were used during domain modelling. Pin fin heat sink orientation and heating power value were changed. Simulations were done for steady state operation. Radiation heat transfer was also accounted and used as a parameter. Same cases were evaluated with and without radiation. Conjugate heat transfer also defined by protecting solid volume of the heat sink and by defining a constant heat flux on the bottom surface of the heat sink. Boussinesq approximation was used for natural convection flow and heat transfer CFD analysis. All thermo-physical properties were assumed constant including the thermal expansion coefficient. The main aim of the work is conducting a feasibility of CFD in this particular arrangement. Rayleigh number of the natural convection flow was changed by differing the heat flux for laminar flow interval. Validation was done by comparing numerically obtained surface temperature values with experimental ones. It is found that upward facing arrangement yield the best thermal performance. Also, accounting radiation heat transfer greatly effects results. Thermal radiation can be up to 25% of thermal convection by assuming maximum emissivity value. However, it is evaluated that reducing emissivity value assumption to a lower number would decrease the percentage of thermal radiation greatly while not changing the trends. CFD is found favourable in respect of natural convection heat transfer from pin fin heat sinks in laminar interval. Nevertheless, there are numerous parameters that should be investigated in terms of numerical options and assumptions, as future work.

CHT-21-274 Development and verification of meshless diffuse approximate method for simulation of single phase, compressible flow in axisymmetry, by *Khush Bakhat Rana, Rizwan Zahoor, Boštjan Mavrič and Božidar Šarler*

The purpose of the present study is to enable meshless Diffuse Approximate Method (DAM) for simulation of single-phase, Newtonian, compressible flow in axisymmetric geometry. DAM is structured by using the second-order polynomial basis functions and the Gaussian weight function, leading to the weighted least squares approximation on overlapping sub-domains. The coupled set of partial differential equations, i.e. mass conservation, momentum conservation, and equation of state, is solved in primitive variables and strong form by using Pressure Implicit with Splitting of Operators (PISO) pressure-velocity coupling on an irregular node arrangement. Implicit time discretization is performed for the predictor step of PISO while in the corrector steps the equations are discretized explicitly. The numerical model is validated for flow in a constant area, axisymmetric tube with helium gas obeying ideal gas law. The solver's accuracy is assessed by investigating the shape of the Gaussian weight and the number of the nodes in the local subdomains. The calculated velocity and pressure fields are compared with Finite Volume Method (FVM) results, obtained by OpenFOAM software. Good agreement has been achieved.

CHT-21-275 Constrained optimization of microchannel cooling systems with and without uncertainty, by *Yogesh Jaluria and Xiaobing Zhang*

Microchannel flows are of interest in the thermal management of electronic systems, microfluidics and biological systems. In thermal management of electronics, microchannel flows are needed to remove high heat fluxes, ranging up to 10^6 W/m² and even higher. In this paper, a microchannel cooling system for a 1 cm x 1 cm electronic chip or component is studied and optimized. Numerical simulations are carried out to study the conjugate heat transfer and flow behavior in the microchannels. Several design variables and operating conditions are considered for acceptable and optimal design. These include channel width or number of channels, geometry of the microchannels, flow rate and heat flux input. Of particular interest are the rate of heat transfer, thermal resistance, pressure drop, pumping power needed, and hot spot temperature. Constraints are imposed on the overall pressure drop and on the maximum temperature of the hot spot. The design and optimization of the system is carried out under these two main constraints. The Polynomial Response Surface (PRS) results with respect to the design variables and operating conditions are obtained. The objective is to reduce both the pumping power and the thermal resistance under hot-spot temperature and required pressure constraints. However, a decrease in thermal resistance is accompanied by an increase in pumping power, leading to an optimization problem. First, the deterministic problem, with fixed parametric values, is considered in detail. Then the uncertainty in these variables is introduced. Uncertainties are often significant in thermal systems. Any minor variations in the design variables or operating conditions may lead to system failure. The standard derivations for the variables are taken as 5-10 % of the mean values. The failure probability is chosen as 0.13%, which is the usually accepted level in reliability studies. With varying weights on the two conflicting objectives, the Pareto frontiers are determined first for the deterministic cases and then with uncertainties. The two results are compared, and the differences demonstrate the importance of uncertainty in obtaining a realistic and satisfactory design. The Pareto frontiers can be used with trade-off to obtain

optimal solutions for given applications. Several cases, with different constraints, are investigated and the results presented and discussed. This study thus provides the means to obtain reliable and realistic design solutions for microchannel cooling systems.

CHT-21-276 Artificial neural network aided multipoint temperature measurement using a grid-shape electric circuit of resistance temperature detectors, by **Runze Mao, Masashi Kishimoto and Hiroshi Iwai**

In-plane multipoint temperature measurement has received more attention due to the increasing need to determine temperature profiles accurately in many electrochemical devices, such as fuel cells, electrolysis cells, and batteries. Since it is difficult to secure an optical path, optical measurement devices such as infrared cameras cannot be used. Contact-type temperature sensors such as thermocouples and resistance temperature detectors (RTDs) are usually applied to perform the multipoint temperature measurement. However, when many thermocouples or RTDs are installed to acquire the temperature distribution, the installation of these sensors requires excessive use of connecting cables, which not only complicates the experimental arrangement but can even affect the temperature field. In this study, a novel method to measure multipoint temperature using a grid-shape circuit constructed with RTDs is proposed with fewer cables attached only at the outer perimeter of the circuit. DC voltage is applied between a set of nodes in the circuit and the voltage of some selected nodes and the response current are measured as outputs. After conducting a few measurements, the obtained data are correlated to the local temperature through the resistances of the RTDs with an assistance of an artificial neural network. The proposed method was validated by conducting multipoint temperature measurements in the temperature range from around 296 K to 358 K. The accuracy estimated from the thermocouple measurements is confirmed 0.5 K.

CHT-21-277 Convergence analysis of steady-state natural convection in a annular cavity filled with porous medium and heated by the inner wall, by **Beatriz Machado dos Santos, Ludimila Silva Salles de Sá and Jian Su**

The present work aims to briefly present the mathematical development and the convergence analysis of an two-dimensional study on the steady-state natural convection in an annulus cavity filled with porous medium and heated by the inner wall, through the generalized integral transform technique (GITT), a well-established hybrid numerical analytical method applicable to the solution of linear or nonlinear convection–diffusion problems, which presents relatively low computational cost. The resulting system of non-linear ordinary differential equations, for temperature and stream function, through performing the GITT is numerically solved by the computational software Mathematica. The convergence of the hybrid solution is demonstrated and a double solution phenomenon for a specific combination of Rayleigh number, angular size and radius ratio of the cavity is presented.

CHT-21-278 Numerical analysis of heat transfer and fluid flow performance in different microchannels heat sink geometries, by **Isabelle Guimarães da Silva**, João Batista Campos Silva and Elaine Maria Cardoso

This work analyzes different materials (aluminum and copper) and geometries of heat sinks, by changing the number of channels, and investigates their influence on the velocity flow field, pressure drop, and heat transfer. The CFD software ANSYS FLUENT® was applied. The water is used as the working fluid. A uniform velocity and temperature (293.15 K) were applied in the inlet of the heat sink. The inlet velocity varied from 0.21 to 0.53 m/s and the Reynolds number based on the hydraulic diameter and inlet velocity varied from 400 to 1000. A heat flux, corresponding to 130 W dissipated power for an Intel Core i7® processor, was applied at the bottom surface of the heat sink. By modifying the solid material, it was possible to obtain different temperature distributions, as well as the pressure drop and the requested pumping power consumption. Comparisons were performed on how the velocity and temperature fields changed according to boundary conditions. The multi-microchannel configuration provides a more uniform wall-temperature distribution; by using copper as heat sink material, the wall temperature decreases around 16% as compared to aluminum. Regardless of the heat sink material, multi-microchannels provide a decrease of around 28% in the wall temperature as compared to the single-channel configuration; even the higher pressure drop observed for the multi-microchannels configuration its effect on the pumping power consumption is acceptable (for the highest Reynolds number, the pressure drop is 512.5 Pa corresponding a pumping power of 4.1 mW). Therefore, the proposed multi-microchannel copper heat sink has a higher cooling performance when compared to the single-channel analyzed in this study.

CHT-21-280 Heat and fluid flow modelling of a high-temperature packed-bed reactor for solar thermochemical energy storage, by **Bo Wang**, Lifeng Li, Florian Schaefer, Apurv Kumar, Vicent M. Wheeler and Wojciech Lipinski

The reduction of iron–manganese oxide particles in a high-temperature packed-bed solar thermochemical reactor is investigated using a transient three-dimensional computational fluid dynamics model. The model couples the reaction kinetics, heat transfer and fluid flow and employs an Eulerian approach to simulate the transport phenomena in the indirectly irradiated packed bed. A reactor prototype is tested under simulated high-flux solar irradiation to validate the model. The validated model is used to evaluate the performance of the reactor. For the baseline case, the calculated temperature profiles indicate that the non-uniform temperature distribution in the start-up phase is later homogenized by the thermal emission of the reactor components at elevated temperatures. When the reaction takes place, the maximum temperature difference in the reactive zone is less than 100 K. The instantaneous peak solar-to-chemical energy efficiency reaches 9.3%. The operating conditions, including the incident flux, sweep gas velocity, and the objective reaction extent for batch replacement, are parametrically studied using the validated model to obtain the optimal solar-to-chemical efficiency. The efficiency increases monotonically with an increasing incident flux and a decreasing sweep gas flow rate. The optimal solar-to-chemical efficiency of 11.4% is reached under an incident flux of 3000 suns and a sweep gas velocity of 0.01 m/s. The objective reaction extent is 95.5% for replacing a new batch of particles. The corresponding processing rate of the iron–manganese particles is 1.3 g/s.

CHT-21-281 Impulsion of space and temperature dependent internal heat generation/absorption on MHD boundary layer slip flow of a nanofluid over a moving plate with induced magnetic field, by *Shahina Akter and M. Ferdows*

The goal of this article is to investigate the combined effects of space and temperature dependent internal heat generation/absorption (non-uniform heat source/sink) on MHD heat transfer flow of an incompressible, viscous and electrically conducting water based nanofluid under the influence of slip over a moving plate with the effect of induced magnetic field. A scaling group of transformation is used to reduce the governing non-linear partial differential equations into a set of non-dimensional ordinary differential equations. The transformed system of differential equations is solved numerically, employing the Spectral relaxation method (SRM) via MATLAB R2018a software. SRM is a simple iteration scheme that does not require any evaluation of derivatives, perturbation, and linearization for solving a non-linear systems of equations. The solutions for the flow and heat transfer characteristics are evaluated numerically for various values of the embedded parameters respectively on motion, induced magnetic field and heat transfer properties are explored through graphs and tables and discussed in details. The skin-friction coefficient and heat transfer rate have also been studied. Three different types of nanoparticles considered are Cu, Ag and TiO₂ by using water-based fluid with Prandtl number Pr=6.2 without any slip condition between them. In order to get the clear insight of the physical problem, the present results are discussed with the help of graphical illustrations for Cu-water. The change in the skin friction coefficient and Nusselt number are higher for large values of ϕ with M. It is also observed that TiO₂ has the highest momentum, magnetic and thermal boundary layer comparing with Cu and Ag.

CHT-21-282 Finite difference solution of bio-magnetic flow of heat transfer over moving horizontal plate by the presence variable viscosity and temperature, by *Sadia Anjum Jumana, M. Ferdows and E.E. Tzirtzilakis*

This research describes the finite difference solution of a 2D, steady, laminar, viscous, incompressible boundary layer and heat transfer flow of a Bio-magnetic fluid over a convectively heated continuously moving horizontal plate in the presence of a magnetic field. All the fluid properties are supposed to be constant, except for the fluid viscosity which is taken as an inverse linear function of temperature. Moreover, the temperature at the wall is assumed to follow the power law variation with the x-coordinate. The solution procedure involves converting the governing system of coupled PDEs (Momentum and Energy equations) into nonlinear ODEs by establishing similarity transformations. The transformed ODEs along with the boundary conditions are then solved numerically by introducing an efficient numerical technique based on the finite difference algorithm. The significant effects of the governing parameters on the flow fields along with the skin friction and heat transfer rate are presented more in details. Verification of this work has been done by comparing the results numerically as well as graphically with former results and quite good agreement is found. It has been analyzed theoretically by using suitable transformations that the ferrohydrodynamic interaction parameter, has a great enhancement on bio-magnetic fluid rather than regular fluid. It is also noticed that the buoyancy force parameter, the viscosity-temperature parameter, and power-law variation in temperature, have significant effects on the flow and

heat transfer mechanism. These outcomes could be of interest in medical as well as bioengineering implementations, like, magnetic drug delivering in blood cells, separating RBCs (Red Blood Cells), controlling the flow of blood during surgeries, treating cancer by producing magnetic hyperthermia etc.

CHT-21-283 Radiative heat transfer in a polydispersion of ceramic particles under high-flux solar irradiation, *by Jingjing Chen, Apurv Kumar, Joe Coventry, Jin-Soo Kim and Wojciech Lipinski*

Solar particle receivers use ceramic particles as the heat transfer and storage medium. They can achieve temperatures over 1000°C due to direct absorption of solar irradiation. Radiative transfer in receivers is complex because of the spectral dependence of the optical and radiative properties of the particles, as well as non-uniform particle size and concentration distributions. An accurate prediction of radiative transfer is desired to understand the radiation–particle interactions. In this work, the particle size effects on radiative and particle–gas convective heat transfer in a system of two infinite parallel plates containing polydisperse particles suspended in air are investigated. The particulate medium is modelled as a non-gray, absorbing, emitting, and anisotropically-scattering medium. The Monte Carlo is used to solve the radiative transfer. The Mie theory is employed to calculate radiative properties. The finite volume method and the explicit Euler time integration scheme are used to solve the energy equation that couples radiative and convective heat transfer. Three models are used to investigate the polydispersity effect: (i) a polydispersion system with multiple particle-size components represented by individual properties and heat transfer rates, (ii) a polydispersion system of a single particle component characterized by a set of properties, and (iii) an approximation monodispersion system. Different models to incorporate particle size effects to radiative and convective heat transfer result in drastic differences in radiative flux and temperature profiles for particle and gas phases. The model of distinguishing particles as the multi-component medium provides insights into size-dependent transport mechanism and thermal response.

CHT-21-284 Heat transfer modelling of an isolated bubble in sodium pool boiling, *by Siddharth Iyer, Apurv Kumar, Joe Coventry and Wojciech Lipinski*

The use of boiling sodium as a heat transfer fluid in a solar thermal receiver is attractive to provide near-isothermal heat for industrial applications. A key challenge that has hindered the development of such a receiver is boiling instability, which manifests itself as excessive superheat followed by flash boiling. Therefore, to stabilize the flow, it is vital to gain a fundamental understanding of the boiling process. As a first step, a reduced-order bubble growth model is developed in this work to study the growth of a single sodium bubble in a liquid pool. The model predicts the growth rate of the bubble based on the heat transferred from several places: a layer of fluid trapped below it called the microlayer, the thermal boundary layer and the bulk liquid surrounding the bubble. A transient 2D conduction equation is solved to model the cooling of the wall below the bubble due to evaporation of the microlayer and the thermal boundary layer. The model is validated against experimental results for water and extended to analyze the relative contribution of different heat transfer mechanisms to the growth of a sodium bubble. It is found that the microlayer heat transfer is the dominant mechanism controlling bubble growth in sodium. A parametric study on the

effect of wall superheat, contact angle and temperature of the bulk liquid showed that the bubble size increases with increasing superheat, contact angle and bulk liquid temperature.

CHT-21-285 Prediction of tortuosity factor of sphere-packing porous media by three-dimensional convolutional neural network, by **Yodai Matsui**, *Masashi Kishimoto and Hiroshi Iwai*

Porous materials are often used for chemical and electrochemical devices, and their three-dimensional structures are important to understand transport and reaction. However, quantification of structural parameters is sometimes numerically expensive. For example, quantification of tortuosity factor, which is used to evaluate effective transport coefficient, requires diffusion simulation in complex porous structures. This can be a bottleneck when we predict performance of various structures and find an optimal structure. Convolutional neural network (CNN) is recently used for image analysis and is expected to reduce computational cost required to estimate structural parameters. In this study, therefore, a CNN model is developed to estimate tortuosity factor of porous structures. Synthetic porous structures are first generated using sphere-packing algorithm, and their tortuosity factors are obtained by conducting diffusion simulation. The obtained dataset is used to train the constructed CNN model. Subsequently, tortuosity factors of unknown structures are predicted by the trained model, and the accuracy is compared with that of the Bruggeman equation, an empirical equation to estimate tortuosity factor. Also, real three-dimensional structures of solid oxide fuel cells (SOFCs) are used to confirm generalization performance of the model. It is found that the performance of the model for synthetic porous structures is higher than that of the Bruggeman equation, while its accuracy for the real structures is insufficient.

CHT-21-287 Integral transform solution of axial-diffusion Graetz-problems in infinite domains: hybrid symbolical-numerical computation, by *N. R. Braga Jr., D. J. N. M. Chalhub and L. A. Sphaier*

A solution of an extended Graetz problem with axial diffusion in an infinite tube with external boundary convective boundary conditions is has been developed. The tube is divided in a preparation upstream region followed by a downstream region, with a step jump in the external convective boundary condition where the regions meet. The solution methodology is based on the Generalized Integral Transform Technique, using Helmholtz problems for the eigenseries expansions. This maintains the calculation of eigenfunctions-related quantities as simple as possible, hence minimizing the amount of necessary computational work. Although the proposed solution is a closed-form analytical one, there are computational steps required for its implementation, some of which involve numerical methods, such as: evaluation of integral coefficients, solution of transcendental equations, calculation of matrix eigenvalues, and the solution of linear systems.

LIST OF PARTICIPANTS

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Luiz ABREU

Rio de Janeiro State University, UERJ
Rua Bonfim, 25 - Vila Amélia
Nova Friburgo, RJ, 28625-570
BRAZIL
Tel: +55 22 99906 3796
E-Mail: abreu.l@gmail.com

Imad AIT LAASRI

Faculty of Sciences Semlalia
Cadi Ayyad University
Laboratory (LaMEE), Marrakesh
Menara, 40000
MOROCCO
Tel: +2126 5787 9912
E-Mail: imadaitlaasri@gmail.com

Mona AL-MQBAS

Technische Universitat Berlin
Jagowstrasse 20, 10555
Berlin
GERMANY
Tel: +49 174 621 5630
E-Mail: m.al-mqbas@tu-berlin.de

Leonardo S.B. ALVES

Rua Passo da Pátria 156
Fluminense Federal University
Bloco E, Sala 216, Niteroi
24210, Rio de Janeiro
BRAZIL
Tel: +212 629 5576
E-Mail: leonardo.alves@gmail.com

Fabiano ALVES DOS SANTOS

Department of Mechanical Engineering
Poli/COPPE Federal University of Rio de Janeiro
PPO Box 68503
Rio de Janeiro, 21941-972
BRAZIL
Tel: +55219 9754 0504
E-Mail: fasantos.rj@gmail.com

Frederic ANDRE

University of Claude Bernard Lyon 1
CNRS, INSA-Lyon
CETHIL
5008 Villeurbanne
FRANCE
Tel: +47 243 8816
E-Mail: frederic.andre@insa-lyon.fr

Gustavo ANJOS

Universidade Federal do Rio de Janeiro
21941-914
Rio de Janeiro
BRAZIL
Tel: +5521 3938 8402
E-Mail: gustavo.rabello@coppe.ufrj.br

Eslem Enis ATAK

ODTÜ Makina Mühendisliği
Middle East Technical University
A-128, 6800
Çankaya/Ankara
TURKEY
Tel: +9053 1772 3905
E-Mail: eatak@metu.edu.tr

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Mohammad AZAD

Dalhousie University
B-30 West Street
NS, B2G 1R8
CANADA
Tel: +90 2870 0279
E-Mail: azadsemail@gmail.com

Seyedmohsen BAGHAEI OSKOUEI

Mechanical Engineering Department
Middle East Technical University

Ankara, 06800
TURKEY
Tel: +90 539 342 8122
E-Mail: seyedmohsen.oskouei@metu.edu.tr

Bantwal R. BALIGA

Department of Mechanical Engineering
McGill University
817 Sherbrooke St. W.
Montreal, Quebec H3A 0C3
CANADA
Tel: +1 514 398 6287
E-Mail: bantwal.baliga@mcgill.ca

Liliane BARICHELLO

Instituto de Matemática e Estatística
Universidade Federal do Rio Grande do Sul
Av Bento Goncalves 9500, Cx Postal 15080 Porto
Rio Grande do Sul, 91509900
BRAZIL
Tel: +5551 3308 6175
E-Mail: LBARIC@MAT.UFRGS.BR

Jean-Luc BATTAGLIA

University of Bordeaux
Nouvelle Aquitaine
33400
FRANCE
Tel: +64 364 7279
E-Mail: jean-luc.battaglia@u-bordeaux.fr

Steven B. BEALE

Forschungszentrum Juelich GmbH
Wilhelm-Johnen-Strasse
Juelich, 52425
GERMANY
Tel: +49 1767 097 6641
E-Mail: s.beale@fz-juelich.de

Rafael BENDIA

Federal University of Rio de Janeiro
Rua Dezenove de Fevereiro, 112
22280030
BRAZIL
Tel: +55 219 8153 9745
E-Mail: rafael.bendia@coppe.ufrj.br

Arunim BHATTACHARYA

Northern Illinois University
871 Regent Dr, Apt 312
Illinois, 60115
USA
Tel: +815 593 6036
E-Mail: Z1776960@students.niu.edu

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Bernardo BUONOMO

Dipartimento di Ingegneria
Università degli Studi Della Campania Luigi Vanvitelli-
Via Roma, 29
Aversa, 81031
ITALY
Tel: +3908 1501 0358
E-Mail: bernardo.buonomo@unicampania.it

Guilherme CAMELO DE FREITAS

Universidade Federal do Rio de Janeiro
Rosa Caride, 45 - Porto Novo
Rio de Janeiro, 24741360
BRAZIL
Tel: +55219 9499 0040
E-Mail: guifrei@gmail.com

Eyüp CANLI

Teknoloji Fakültesi, Makine Muhendisligi Bolumu
Selcuk University
Selcuklu
Konya, 42130
TURKEY
Tel: +90 507 231 2828
E-Mail: ecanli@selcuk.edu.tr

Victor CARLOS TEIXEIRA

ABCM
Alameda Jose Faciola, 21, apto 1707
Parei, 66040170
BRAZIL
Tel: +919 8416 2929
E-Mail: victorteixeira@mecanica.coppe.ufrj.br

Rodrigo CASTELLO BRANCO

Pontifícia Universidade Católica do Rio de Janeiro
R. Marques de S. Vicente 225
Rio de Janeiro, 22453-900
BRAZIL
Tel: +55219 7216 8054
E-Mail: rodrigofcbranco@hotmail.com

Evgeniy CHEBAKOV

Moscow Aviation Institute

Moscow, 125993
RUSSIA
Tel: +792 5070 4728
E-Mail: ChebakovEvgeny@yandex.ru

Jingjing CHEN

The Australian National University
35A Science Road
Canberra, ACT, 2601
AUSTRALIA
Tel: +40 657 1753
E-Mail: jingjing.chen1@anu.edu.au

Janhavi CHITALE

Florida International University
9120 SW 137th Avenue, Apt. 1222
FL, 33186
USA
Tel: +267 772 3609
E-Mail: jchit002@fiu.edu

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Yanki ÇOBANOĞLU

Mechanical Engineer Department
Middle East Technical University

Ankara, 06800

TURKEY

Tel: +90 506 254 6787

E-Mail: yankicob@gmail.com

Pedro J. M. COELHO

Departamento de Engenharia Mecânica
Instituto Superior Técnico
Secção de Termoflúidos e Energia Av Rovisco Peis
1049 001 Lisbon

PORTUGAL

Tel: +3512 1841 7186

E-Mail: pedro.coelho@tecnico.ulisboa.pt

Marcelo COLACO

Rua Miguel Lemos 99, apt. 303
Federal University of Rio de Janeiro

Rio de Janeiro, 22071000

BRAZIL

Tel: +55 219 8848 9483

E-Mail: colaco@ufrj.br

Juliana COSTA

Federal University of Rio de Janeiro
Rua Rio Engenho Novo, 5, casa 2 - Taquara
22713-571,RJ

BRAZIL

Tel: +219 6995 7123

E-Mail: julianacsssilva@poli.ufrj.br

Renato COTTA

Pem/Coppe/Ufrj-Cidade Universitaria
Univ. Federal de Rio de Janeiro
Cx postal 68503, 21945-970
Rio de Janeiro-RJ

BRAZIL

Tel: +5521 2562 8566

E-Mail: cotta@mecanica.coppe.ufrj.br

Dezhi DAI

Nuclear Science and Engineering Division
Argonne National Laboratory

Lemont, IL, 60559

USA

Tel: +682 375 0534

E-Mail: daid@anl.gov

Carlos Eduardo DALLA

Universidade Federal do Espirito Santo
Av. Saturnino de Britto, n 1350
Espirito Santo,29055-180

BRAZIL

Tel: +55 027 99278 5011

E-Mail: carloseduardodalla@gmail.com

Renato DE OLIVEIRA

Universidade Federal do Rio de Janeiro
25655350
Rio de Janeiro

BRAZIL

Tel: + 55249 9227 0962

E-Mail: renato.rosa@poli.ufrj.br

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Ludimila DE SA

COPPE
Rua Dona Romana, 20710-200
RJ
BRAZIL
Tel: +219 8194 2684
E-Mail: ludimilasalles.md@coppe.ufrj.br

Santiago del RIO OLIVEIRA

Uni. Estadual Paulista "Julio de Mesquita Filho"-UNESP

Sao Paulo
BRAZIL
Tel: +17033 360
E-Mail: santiago.oliveira@unesp.br

Leonid A. DOMBROVSKY

Joint Institute for High Temperatures
Russian Academy of Sciences
Krasnokazarmennaya 17 A, NCHMT
111116 Moscow
RUSSIA
Tel: +7 910 408 0186
E-Mail: ldombr@yandex.ru

Juliana DREYER

Federal University of Rio de Janeiro, UFRJ
Rua Marques de Parana, 49
22230-030,RJ
BRAZIL
Tel: +55 219 8090 2032
E-Mail: dreyer.juliana@poli.ufrj.br

Milorad DZODZO

1000 Westinghouse Dr.
Westinghouse Electric Company
16066
PA
USA
Tel: +141 2979 4558
E-Mail: dzodzomb@westinghouse.com

Olivier FARGES

LEMETA, Lorraine University
2 Avenue de la Forêt de Haye
Vandœuvre-lès-Nancy, 54500
FRANCE
Tel: +333 7274 4283
E-Mail: olivier.farges@univ-lorraine.fr

Kunio FUJIWARA

Osaka University
565-0871
Osaka
JAPAN
Tel: +816 6879 7312
E-Mail: k.fujiwara@mech.eng.osaka-u.ac.jp

Alexander GELFGAT

School of Mechanical Engineering
Tel-Aviv University
Ramat Aviv
69978, Tel-Aviv
ISRAEL
Tel: +972 3640 7207
E-Mail: gelfgat@tau.ac.il

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Bruno GOFFERT

Pr Mal Eduardo Gomes, 50
Instituto Tecnológico de Aeronáutica
Sao Jose dos Campos
São Paulo, 12228-900
BRAZIL
Tel: +5511 97552 4885
E-Mail: bruno.goffert@gmail.com

Fernando GROFF

Programa de Pós-Graduação em Matemática Aplicada
Universidade Federal do Rio Grande do Sul
Av. Bento Gonçalves, 9500, Prédio 43111
Rio Grande do Sul, 91509900
BRAZIL
Tel: +5551 3308 6213
E-Mail: fernando.groff@ufrgs.br

Isabelle GUIMARAES da SILVA

Campus of Sao Joao da Boa Vista
UNESP, Sao Paulo State University
School of Engineering
Ilha Solteira, SP, 15385 000
BRAZIL
Tel: +119 9940 3119
E-Mail: isabelle.g.silva@unesp.br

Nursel GÜLER

Mechanical Engineering Department
Middle East Technical University
D-104
06800, Ankara
TURKEY
Tel: +90 312 210 2541
E-Mail: nursel@ichmt.org

Joao Paulo INNOCENTE DE SOUZA

Universidade Federal do Rio de Janeiro
Travessa Plácido de Castro, 106
Rio de Janeiro, 21060-220
BRAZIL
Tel: +55 219 8715 5761
E-Mail: jpisouza@mecanica.coppe.ufrj.br

Siddharth IYER

Australian National University
Craig Building 35A, North Road
ACT, 2601
AUSTRALIA
Tel: +46 835 8385
E-Mail: siddharth.iyer@anu.edu.au

Bruno JACCOUD

Federal University of Rio de Janeiro, UFRJ
Estrada do Barro Vermelho, 484 - BL1 APTO 1306
Rio de Janeiro, 21540500
BRAZIL
Tel: +55 219 7202 0056
E-Mail: bruno.jaccoud@mecanica.coppe.ufrj.br

Yogesh JALURIA

Department of Mechanical Engineering
Rutgers University
98 Brett Rd.
Piscataway, NJ 08854
U.S.A.
Tel: +1 732 445 3652
E-Mail: jaluria@soe.rutgers.edu

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Charles JANEKE

Constellation Dynamics/QUASAR
1330 Ingraham St 114, Los Angeles
CA, 90017
USA
Tel: +213 880 1454
E-Mail: charljaneke@gmail.com

Ibrahim JARRAH

104 S Wright St, 216 Talbot Laboratory
University of Illinois Urbana-Champaign
Urbana
Illinois, 61801
USA
Tel: +217 333 2295
E-Mail: ijarrah2@illinois.edu

Sambhaji KADAM

Texas A and M University at Qatar
Education City
Doha, 23874
QATAR
Tel: +974 3312 0620
E-Mail: sambhaji.kadam@qatar.tamu.edu

Sung Yeon KIM

Sungkyunkwan University
2066, Seobu-ro, Jangan-gu, Suwon-si
Gyeonggi-do, 16419
SOUTH KOREA
Tel: +3210 3130 6927
E-Mail: ksy203@skku.edu

Peter KLEIN

Council for Scientific and Industrial Research
Meiring Naude Road, Pretoria
Gauteng, 81
SOUTH AFRICA
Tel: +271 2841 4132
E-Mail: pklein@csir.co.za

Tania KLEIN

NBPD, LabCFD
Federal University of Rio de Janeiro
Av. Athos da Silveira Ramos, 149, Bloco E
Rio de Janeiro, 21941-909
BRAZIL
Tel: +219 8624 1999
E-Mail: tania@eq.ufrj.br

Jan KREN

Reactor Engineering Division
Jozef Stefan Institute

Ljubljana, 1000
SLOVENIA
Tel: +386 4026 6924
E-Mail: jan.kren@ijs.si

Benno KRUEGER

Technische Universität Darmstadt
Alarich-Weiss-Strate 10
Hessen, 64283 Darmstadt
GERMANY
Tel: +4917 8558 9206
E-Mail: krueger@ttd.tu-darmstadt.de

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Afef LARIBI

Laboratoire Femto-St.
Belfort, 90000
FRANCE
Tel: +337 261 2216
E-Mail: afef.laribi@univ-fcomte.fr

Anatoliy LEVIN

Melentiev Energy Systems Institute
Lermontova 130, Irkutsk oblast
664033
RUSSIA
Tel: +790 8668 1499
E-Mail: lirt@mail.ru

Bruna LOIOLA

Praca General Tiburcio, 80, Praia Vermelha, URCA
Instituto Militar de Engenharia
22290-270
Rio de Janeiro
BRAZIL
Tel: +55 219 6504 0573
E-Mail: bruna.loiola@ime.eb.br

Beatriz MACHADO DOS SANTOS

Federal University of Rio de Janeiro
Rua Paula e Silva, 32 São Cristóvão
Rio de Janeiro, 20910120
BRAZIL
Tel: +2198 856 3542
E-Mail: bmachado@coppe.ufrj.br

Denis MAILLET

Universite de Lorraine
Grand Est.
54505
FRANCE
Tel: +33 68 345 4689
E-Mail: denis.maillet@univ-lorraine.fr

Amit MAKHIJA

5, Gordhan Dham Nagar, Ujjain
Indian Institute of Technology Palakkad
Madhya Pradesh
456010
INDIA
Tel: +958 409 7862
E-Mail: makhijaamit0909@gmail.com

Oronzio MANCA

Dipt.di Ingegneria Industriale e dell'Informazione
Seconda Universita degli Studi di Napoli
Via Roma 29
Aversa (CE) ,81031
ITALY
Tel: +39 081 501 0217
E-Mail: oronzio.manca@unina2.it

Runze MAO

Kyoto University
615-8540, Kyoto
JAPAN
Tel: +81 075 383 3652
E-Mail: mao.runze.67r@st.kyoto-u.ac.jp

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Bruno Henrique MARQUES MARGOTTO

PEM/COPPE

Universidade Federal do Rio de Janeiro

Rua Coronel Joao Olintho, 233 AP 302

Rio de Janeiro

BRAZIL

Tel: +55 27 99710 0133

E-Mail: brunohmmargotto@gmail.com

Krishna Reddy MARYADA

The University of Auckland

20 Symonds Street, Auckland CBD

Auckland

NEW ZEALAND

Tel: +642 7216 6844

E-Mail: kmar699@aucklanduni.ac.nz

Massoud MASSOUDI FAIRD

CIC Virtuhcon

Technische Universität Bergakademie Freiberg

Haus 1, EVT, Fuchsmühlenweg 9D

Sachsen,9599

GERMANY

Tel: +373 139 4496

E-Mail: massoud.massoudi-farid@iec.tu-freiberg.de

Yodai MATSUI

Kyoto University

301 Purando-ru 17-3 Katsura Nozatocho Nishikyo-ku

Kyoto-shi, 615-8073

JAPAN

Tel: +81 80 6123 8754

E-Mail: matsui.yodai.74r@st.kyoto-u.ac.jp

George MEMOS

NCSR Demokritos

Institute of Nanoscience and Nanotechnology

Agia Paraskevi Attikis, P.O.Box 60037

15310, Arhens

GREECE

Tel: +30 210 650 3238

E-Mail: g.memos@inn.demokritos.gr

Francisco MILLER

Federal University of Rio de Janeiro

Rua Riachuelo, 169 apt 804 Centro Rio de Janeiro

Rio de Janeiro, 20230-010

BRAZIL

Tel: +55 21 97101 2848

E-Mail: franc.miller@mecanica.coppe.ufrj.br

Roman MIRONOV

ORPE "Technologiya" named after A.G.Romashin

84/6, Hvoynaya st. Obninsk.,Kaluzhskaya oblast'

249037

RUSSIA

Tel: +795 3462 9794

E-Mail: manarom@yandex.ru

Abdulmajeed MOHAMAD

University of Calgary

220 Brown Bear Point, Alberta

T4C0B5

CANADA

Tel: +140 3680 2112

E-Mail: mohamad@ucalgary.ca

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

M.S. NAARENDHARAN

NIT Tiruchirappalli
233 MIED, IIT
Roorkee, 247667
INDIA
Tel: +9113 3228 4781
E-Mail: msnaaren@gmail.com

Carolina NAVEIRA-COTTA

AV Athos da Silveira Ramos, s/n, CT
COPPE/UFRJ
21945-970
Rio de Janeiro
BRAZIL
Tel: +21 98801 2330
E-Mail: carolina@mecanica.coppe.ufrj.br

Angela NIECKELE

PUC-Rio

Rio de Janeiro
BRAZIL
Tel: +22451900
E-Mail: nieckele@puc-rio.br

Perumal NITHIARASU

College of Engineering
Swansea University
Singleton Park
Swansea, Wales SA1 8EN
U.K.
Tel: +4479 7915 6116
E-Mail: P.Nithiarasu@swansea.ac.uk

Carlos NOBREGA

rua do imperador 971
CEFET-Petropolis
Rio de Janeiro
25620-003
BRAZIL
Tel: +219 6722 1967
E-Mail: nobrega@pobox.com

Carlo NONINO

Polytechnic Department of Engineering and Architecture
Universita degli Studi di Udine
via delle Scienze 206
33100 Udine
ITALY
Tel: +39 0432 55 80 19
E-Mail: carlo.nonino@uniud.it

Andrzej J. NOWAK

Institute of Thermal Technology
Silesian University of Technology
Akademicka 2A
44100
POLAND
Tel: +483 2237 1025
E-Mail: andrzej.j.nowak@polsl.pl

Felipe NUNES

Federal University of Rio de Janeiro
Doutor Paulo Cesar, 87, bl3 ap1506
RJ, 24240-000
BRAZIL
Tel: +219 9584 6004
E-Mail: fsantannan@gmail.com

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Arundas ODUNGAT

IIT PALAKKAD

Kerala, 678623

INDIA

Tel: +944 767 4658

E-Mail: 132104001@smail.iitpkd.ac.in

Tuba OKUTUCU-ÖZYURT

Energy Institute, No: 318, Renewable Energy Division

Istanbul Technical University

Ayazaga Campus, Maslak

Istanbul, 34469

TURKEY

Tel: +90 535 941 7621

E-Mail: okutucuozyurt@itu.edu.tr

Helcio ORLANDE

Dept. of Mechanical Engineering

Federal University of Rio de Janeiro

Cid. Univ., Cx Postal 68503

Rio de Janeiro

BRAZIL

Tel: +55 21 3938 8405

E-Mail: helcio@mecanica.coppe.ufrj.br

Cesar Cunha PACHECO

Federal Fluminense University

R. Passo da Pátria, 152-470

24220-900

BRAZIL

Tel: +55 219 9984 1856

E-Mail: cesarp@id.uff.br

Jacques PADET

ITHEMM - Faculte des Sciences

Universite de Reims

51687

Reims

FRANCE

Tel: +3303 2688 2528

E-Mail: jacques.padet@univ-reims.fr

George PAPADAKIS

South Kensington Campus

Imperial College London

Dept. of Aeronautics

London, SW7 2AZ

U.K.

Tel: +4420 7594 5080

E-Mail: g.papadakis@ic.ac.uk

Vikas Ramesh PATIL

ETH Zurich

Sonneggstrasse 3, ML J43

Zurich, 8092

SWITZERLAND

Tel: +417 8790 0314

E-Mail: vpatil@ethz.ch

Rafaela PEDRASSANI

Universidade Federal do Rio de Janeiro

22040002

Rio de Janeiro

BRAZIL

Tel: +499 9806 6008

E-Mail: rafaela.pedrassani@coppe.ufrj.br

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Lea PENAZZI

IMT Mines Albi
Tarn, Occitanie
81000
FRANCE
Tel: +336 7333 6565
E-Mail: lea.penazzi@mines-albi.fr

Isabela PINHEIRO

Universidade Federal Fluminense
Rio de Janeiro
2441240
BRAZIL
Tel: +55219 9727 2259
E-Mail: isabelaflorindo@id.uff.br

Onur POLAT

Mechanical Engineering Department
Middle East Technical University

Ankara, 06800
TURKEY
Tel: +90 542 635 1016
E-Mail: polat.onur@metu.edu.tr

Carlos Eduardo POLATSCHEK KOPPERSCHMIDT

Rua Guaicurus
Universidade Federal do Rio de Janeiro
n192, Lagoa do Meio, Linhares
Esperito Santo, 29904010
BRAZIL
Tel: +55 279 9928 8833
E-Mail: cadupolkop@gmail.com

Tomas QUIRINO

Department of Mechanical Engineering
Federal University of Rio de Janeiro
Avenida Adolpho de Vasconcelos, 497/904
Rio de Janeiro, 22793380
BRAZIL
Tel: +55 219 9304 6582
E-Mail: tomas.quirino@mecanica.coppe.ufrj.br

Khush Bakhat RANA

Faculty of Mechanical Engineering
University of Ljubljana
AkerA• eva Cesta 6
Ljubljana, 1000
SLOVENIA
Tel: +386 3076 6353
E-Mail: khush.bakhat.rana@fs.uni-lj.si

Hrishiraj RANJAN

Indian Institute of Engineering Science and
West Bengal, 711103
INDIA
Tel: +9187 8982 5035
E-Mail: hrishi.ssec@gmail.com

Alex ROYER

Universite de Lorraine - LEMTA
2 avenue de la Foret de Haye BP 90161 Vandoeuvre-
Grand Est, 54505
FRANCE
Tel: +336 6243 7376
E-Mail: alex.royer@univ-lorraine.fr

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Sarah SANT'ANNA

UFRJ
25935614
Rio de Janeiro
BRAZIL
Tel: +2196 770 6699
E-Mail: saraholiveira@poli.ufrj.br

Daniel SANTOS

Universidade Federal do Rio de Janeiro
Rua Barão de Guaratiba 106
Rio de Janeiro, 22211150
BRAZIL
Tel: +719 9221 3600
E-Mail: daniel.barbedo@coppe.ufrj.br

Fabio SANTOS

Federal University of Rio de Janeiro

Rio de Janeiro, 21941-909
BRAZIL
Tel: +55219 9472 6988
E-Mail: fsantos@eq.ufrj.br

Menekse SENYIGIT

Department of Physics
Ankara University
Tandogan
Ankara, 6100
TURKEY
Tel: +90 546 887 8634
E-Mail: meneksek@science.ankara.edu.tr

Dinesh Kumar SHARMA

Plot No A4, Model Town, Agra Road
Malaviya National Institute of Technology

Rajasthan, 302031
INDIA
Tel: +76 6561 7050
E-Mail: 2019ren9015@mnit.ac.in

Amit Kumar SHAW

Academy of Scientific and Innovative Research

Ghaziabad-201002
INDIA
Tel: +9174 3910 2903
E-Mail: amitkumar.shaw@csio.res.in

Rodrigo SILVA

Federal University of Rio de Janeiro
114 Pereira Nunes Street
Rio de Janeiro, 20540132
BRAZIL
Tel: +55219 7172 3944
E-Mail: rodrigo.silva@mecanica.coppe.ufrj.br

Nilton SILVA

Faculdade De Tecnologia
UFRJ / UFAM
Av. General Rodrigo Otavio, 6200, Coroado, Setor Norte
Amazonas, 69080900
BRAZIL
Tel: +55 929 8245 5703
E-Mail: niltonps@ufam.edu.br

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Terrence SIMON

University of Minnesota
111 Church St S.E. Minneapolis
55455, Minnesota
USA
Tel: +651 503 5652
E-Mail: simon002@umn.edu

Ashutosh Kumar SINGH

Faculty quarters NIT
National Institute of Technology Manipur
Manipur Langol, Imphal
Manipur, 795004
INDIA
Tel: +875 058 4502
E-Mail: as13031996@gmail.com

Vladimir P. SOLOVJOV

Brigham Young University
3301 Shadowbrook Circle, Provo
Utah, 84604
U.S.A.
Tel: +801 422 6543
E-Mail: lemberg.v@gmail.com

Adam SOUSA

Universidade Federal do Rio de Janeiro
25550-170
Rio de Janeiro
BRAZIL
Tel: +91 99155 0698
E-Mail: adamrsousa@gmail.com

Sergio SOUZA

Universidade Federal da Para-ba - UFPB
Rua Marieta Steimbach Silva, 51, AP 1004 B
PB,58043-320
BRAZIL
Tel: +55 8398 851 2466
E-Mail: sergio@mat.ufpb.br

Leandro SPHAIER

Universidade Federal Fluminense
Rua Passo da Patria 156, sala 302, bloco D. Niteroi
23220-320, RJ
BRAZIL
Tel: +55 219 9134 4651
E-Mail: lasphaier@id.uff.br

Joseph SQUEO

University of Connecticut
Dakota Drive Hopewell Junction
NY, 12533
USA
Tel: +845 430 0451
E-Mail: Joseph.squeo@ucon.edu

Shreyas Rohit SRINIVAS

CIC Virtuhcon
Technische Universitat Bergakademie Freiberg
Fuchsmahlenweg 9
09599 Freiberg
GERMANY
Tel: +49 176 3130 8515
E-Mail: Shreyas-Rohit.Srinivas@iec.tu-freiberg.de

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Peter STEPHAN

TU Darmstadt
Alarich Weiss Str. 10
64287 Darmstadt
GERMANY
Tel: +49 6151 162 2260
E-Mail: pstephan@ttd.tu-darmstadt.de

Jian SU

Dept.de Eng.Mechanica e Materiais
Universidade Federal do Rio de Janeiro
PEN/COPPE/UFRJ, CP68509
Rio de Janeiro,21941-972
BRAZIL
Tel: +55219 8231 8996
E-Mail: sujianufrj@gmail.com

Anshul SURI

Indian Institute of Technology Roorkee
50,New Vijay Nagar
Punjab, 144001
INDIA
Tel: +9194 1717 6284
E-Mail: surianshul1@gmail.com

Çiğdem SUSANTEZ

Mechanical Engineering Department
Trakya University
Edirne, 22030
TURKEY
Tel: +9054 3310 8376
E-Mail: cigdemsusantez@trakya.edu.tr

Ilker TARI

Department of Mechanical Engineering
Middle East Technical University
E-104, Çankaya
06800, Ankara
TURKEY
Tel: +312 210 2551
E-Mail: itari@metu.edu.tr

Kazuya TATSUMI

Department of Mechanical Eng. and Science
Kyoto University
Kyotodaigaku-katsura, Nishikyo-ku
Kyoto, 6158540
JAPAN
Tel: +817 5383 3606
E-Mail: tatsumi@me.kyoto-u.ac.jp

Ahmed TEAMAH

McMaster University
57 Mericourt Road, 212
ON, L8S 2N5
CANADA
Tel: +0905 920 6960
E-Mail: teamaha@mcmaster.ca

Victoria TIMCHENKO

School of Mech & Manuf. Engineering
University of New South Wales
2052
Sydney NS Wales
AUSTRALIA
Tel: +614 1285 4148
E-Mail: v.timchenko@unsw.edu.au

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Svetlana TKACHENKO

Department of Mechanical Engineering
University of New South Wales
Kensington, 2033
Sydney
AUSTRALIA
Tel: +41 310 3059
E-Mail: svetlana.tkachenko@unsw.edu.au

Inoussa TOUGRI

Ecole Polytechnique de Ouagadougou (EPO)
Kadiogo (Ouagadougou)
18 BP 143 Ouaga 18
BURKINA FASO
Tel: +226 7183 6718
E-Mail: i.tougri@mecanica.coppe.ufrj.br

Nicolas TRICARD

University of Connecticut
24 Olsen Dr., Mansfield
CT, 06250-1125
USA
Tel: +860 989 6822
E-Mail: nicolas.tricard@uconn.edu

Claudio TUCCI

Universite degli Studi del Molise
Via Francesco De Sanctis 1
Campobasso, 86100
ITALY
Tel: +3933 8812 7882
E-Mail: c.tucci1@studenti.unimol.it

Shota UCHIDA

SCREEN Holdings Co., Ltd.
Osaka University

Kyoto, 612-8486
JAPAN
Tel: +8175 931 7925
E-Mail: sh.uchida@screen.co.jp

Yoshitaka UEKI

Osaka University
2-1 Yamadaoka, Suita
Osaka, 565-0871
JAPAN
Tel: +816 6879 4987
E-Mail: ueki@mech.eng.osaka-u.ac.jp

S. Pratap VANKA

Dept. of Mech. & Ind. Engineering
University of Illinois
1206 W. Green Street, Urbana
IL 61801-3028
U.S.A.
Tel: +1 217 244 8388
E-Mail: spvanka@illinois.edu

Alexey VIKULOV

National Research University
Moscow Aviation Institute
Volokolamskoe shosse, 4
Moscow, 125993
RUSSIA
Tel: +790 3284 8211
E-Mail: vikulovag81@gmail.com

List of Participants
8th Int. Symposium on Advances in Computational Heat Transfer, CHT-21

Bo WANG

The Australian National University
49/8 Baudinette CC
ACT, 2617
AUSTRALIA
Tel: +614 0616 5042
E-Mail: bo.wang@anu.edu.au

Brent W. WEBB

Brigham Young University
A-387 ASB, Provo
UT, 84602
U.S.A.
Tel: +1 801 422 6543
E-Mail: webb@byu.edu

Michael WILD

ETH Zürich
Sonneggstrasse 3
Zürich, 8092
SWITZERLAND
Tel: +414 4632 5445
E-Mail: michaelwild@ethz.ch

Seokbeom YUN

Sungkyunkwan University
2066, Seobu-ro, Jangan-gu, Suwon-si
Gyeonggi-do, 16419
SOUTH KOREA
Tel: +3210 3376 3970
E-Mail: ysb1047a@skku.edu

Mohammed ZAMOUM

Avenue de l'Indépendance
Université M'hamed Bougara de Boumerdes
Boumerdes, 35000
ALGERIA
Tel: +2135 5226 4618
E-Mail: m.zamoum@univ-boumerdes.dz

Xinyu ZHAO

University of Connecticut
191 Auditorium Rd Unit 3139
Connecticut, 6269
USA
Tel: +01 860 486 0241
E-Mail: xinyu.zhao@uconn.edu