Vacuum Science and Technology Division
Fachverband Vakuumphysik und Vakuumtechnik (VA)

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Overview of Invited Talks and Sessions

(Lecture hall HSZ 301)

Invited Talks

VA 1.1	Mon	9:30–10:10	HSZ 301	**Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics** — •Stylianos Varoutis, Christos Tantos, Christian Day
VA 2.1	Mon	12:30–13:10	HSZ 301	**Vacuum Solutions for Dilution Refrigerators** — •Stefan Lausberg

Invited talks of the joint symposium SYSD

See SYSD for the full program of the symposium.

SYSD 1.1	Mon	9:30– 9:55	HSZ 02	**Disentangling transport in topological insulator thin films down to the nanoscale** — •Felix Lüpke
SYSD 1.2	Mon	9:55–10:20	HSZ 02	**Spintronics with Terahertz Radiation: Probing and driving spins at highest frequencies** — •Tom Sebastian Seifert, Tobias Kampfrath
SYSD 1.3	Mon	10:20–10:45	HSZ 02	**Non-radiative voltage losses in organic solar cells** — •Johannes Benduhn
SYSD 1.4	Mon	10:45–11:10	HSZ 02	**Multivalent ions for tuning the phase behaviour of protein solutions** — •Olga Matsarskaia
SYSD 1.5	Mon	11:10–11:35	HSZ 02	**Network Dynamics under Constraints** — •Malte Schröder
SYSD 1.6	Mon	11:35–12:00	HSZ 02	**Exciton spectroscopy of van der Waals heterostructures** — •Philipp Nagler

Invited talks of the joint symposium SYES

See SYES for the full program of the symposium.

SYES 1.1	Thu	9:30–10:00	HSZ 02	**Understanding the physical variables driving mechanosensing** — •Pere Roca-Cusachs
SYES 1.2	Thu	10:00–10:30	HSZ 02	**Mechanics of life: Cellular forces and mechanics far from thermodynamic equilibrium** — •Timo Betz
SYES 1.3	Thu	10:30–11:00	HSZ 02	**A hydrodynamic approach to collective cell migration in epithelial tissues** — •Jaume Casademunt
SYES 1.4	Thu	11:15–11:45	HSZ 02	**The spindle is a composite of two permeating polar gels** — David Oriola, Benjamin Dalton, Franziska Decker, Frank Julicher, •Jan Brugues
SYES 1.5	Thu	11:45–12:15	HSZ 02	**Adding magnetic properties to epitaxial graphene** — •Rodolfo Miranda
SYES 2.1	Thu	15:00–15:30	HSZ 01	**Interactions in assemblies of surface-mounted magnetic molecules** — •Wolfgang Kuch
SYES 2.2	Thu	15:30–16:00	HSZ 01	**Towards phononic circuits based o optomechanics** — •Clivia M. Sotomayor-Torres
SYES 2.3	Thu	16:00–16:30	HSZ 01	**Optical properties of 2D materials and heterostructures** — •Janina Maultzsch

SYES 2.4	Thu	16:45–17:15	HSZ 01	**Bringing nanophotonics to the atomic scale** — •Javier Aizpurua
SYES 2.5	Thu	17:15–17:45	HSZ 01	**Infrared signatures of the coupling between vibrational and plasmonic excitations** — •Annemarie Pucci

Sessions

VA 1.1–1.4	Mon	9:30–11:30	HSZ 301	**Rarefied gas flows and novel approaches for particle simulation**
VA 2.1–2.2	Mon	12:30–13:30	HSZ 301	**Vacuum technology: New developments and applications**
VA 3	Mon	13:30–14:30	HSZ 301	**Annual General Meeting**

Annual General Meeting of the Vacuum Science and Technology Division

Monday 13:30–14:30 HSZ 301

- Bericht
- Wahl
- Verschiedenes

VA 1: Rarefied gas flows and novel approaches for particle simulation

Time: Monday 9:30–11:30 Location: HSZ 301

Invited Talk VA 1.1 Mon 9:30 HSZ 301

Deterministic and stochastic numerical approaches in Rarefied Gas Dynamics — •Stylianos Varoutis, Christos Tantos, and Christian Day — Karlsruher Institut für Technologie (KIT), Institut für Technische Physik (ITEP), Karlsruhe, Germany

During the last decade research in the field of rarefied gas dynamics has attracted a lot of attention. This refreshed interest is due to applications in the emerging field of nano- and micro-fluidics, as well as to the more traditional fields of vacuum technology and high altitude aerodynamics. Some of these applications may include important phenomena such as those related to polyatomic gases, chemical reactions, evaporation and condensation. The gas rarefaction is specified by the Knudsen number (Kn), which is defined as the ratio of the mean free path over a characteristic length of the problem. In general, when the flow is considered as far from local equilibrium, then the well-known Navier-Stokes equations are not valid anymore. In this case, two main numerical approaches can be implemented. The first approach is based on the kinetic theory of gases as expressed by the Boltzmann equation or its associated kinetic models, in which a deterministic numerical solution is performed. The second approach is the Direct Simulation Monte Carlo (DSMC) method. Within the above framework, the first part of this talk will be devoted to the presentation of the aforementioned numerical approaches, while the second part will be devoted to the presentation of illustrative examples, as for instance, the modelling of the particle exhaust of a nuclear fusion reactor and the numerical modelling of a cryopump.

VA 1.2 Mon 10:10 HSZ 301

Deterministic modeling of neutral gas flows in tokamak nuclear fusion devices — •Christos Tantos, Stylianos Varoutis, and Christian Day — Karlsruhe Institute of Technology, Institute for Technical Physics, Karlsruhe, Germany

Over the last few years much effort has been invested in modeling the complex geometry of the divertor region in tokamak fusion devices. Depending on the upstream plasma conditions, the flow reference Knudsen number, defined as the ratio of the mean free path over a characteristic length, may vary over a wide range. The rarefied flow behavior in these systems cannot be properly captured by the typical Navier-Stokes-Fourier approach and must be described by the integro-differential Boltzmann equation or reliable kinetic model equations. The Discrete Velocity Method (DVM) has been developed into one of the most common techniques for solving the Boltzmann equation and the kinetic models. As it is well known simulating multidimensional rarefied gas problems based on the Boltzmann equation is computationally time consuming. Therefore, successful implementation of reliable kinetic models in such problems is important. In the present work the well-established Shakhov kinetic model supplemented by the DVM method is applied to predict the behavior of the neutral gas flow in the divertor region. Results are presented for He and D2 covering a wide range of the involved parameters. Several comparisons between the present deterministic modeling and the stochastic Direct Simulation Monte Carlo are shown and discussed.

20 min. break

VA 1.3 Mon 10:50 HSZ 301

Stochastic Simulation of Mercury Diffusion Pumps Using Direct Simulation Monte Carlo — •Tim Teichmann and Thomas Giegerich — Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

Currently, a continuously working pump train for DEMO (the European demonstration fusion power plant) is under active development. Mercury driven diffusion pumps have been chosen as possible candidates for the high vacuum pumping of the exhaust gases. In order to design and optimize diffusion pumps for DEMO, a reliable numerical simulation method is required.

The numerical simulation of the DEMO diffusion pumps is a complex challenge as the gas flow in the pump spans a wide Knudsen number range. Typical inlet pressures of the diffusion pumps for DEMO are expected to be in the order of 10^{-3} Pa during dwell and up to 1 Pa during burn respectively. This is equivalent to estimated Knudsen numbers in the range of 10 to 0.01. As the Navier-Stokes equations lose their validity at $Kn > 0.1$, classic continuum solvers cannot be applied to the problem at hand. Therefore, the Boltzmann equation has to be solved to describe this flow regime. In this case the Direct Simulation Monte Carlo (DSMC) method was chosen to solve the Boltzmann equation.

The application of DSMC for simulating the DEMO diffusion pumps will be discussed. Additionally, an outlook on possible hybrid simulation techniques will be given.

VA 1.4 Mon 11:10 HSZ 301

IFMIF-DONES gas flow modelling using Test Particle Monte-Carlo Simulations — •Volker Hauer and Christian Day — Karlsruhe Institute of Technology, Institute for Technical Physics, Karlsruhe, Germany

IFMIF, the International Fusion Materials Irradiation Facility, is a test facility for materials foreseen in fusion reactors. High neutron fluxes are generated with an energy spectrum and intensity similar to the conditions at the burn phase inside a fusion reactor. The high energy neutrons result from accelerating deuterons onto a lithium target.

Simulations of the gas flow inside the IFMIF-DONES vacuum system were performed with the Test Particle Monte-Carlo code Molflow+. The IFMIF-DONES model is based on the latest design and of the LIPAc accelerator, which is being built for testing IFMIF accelerator components. Both, LIPAc and IFMIF-DONES share the same type of accelerator subsystems.

The model was prepared for simulation by adding different sets of boundary conditions for the pumping of deuterium and hydrogen originating from beam losses and outgassing, respectively.

The simulations of the gas pumping show pressure profiles which are mainly determined by the beam losses in this subsystem except for the Linac modules where the beam losses are very low. As LIPAc and IFMIF-DONES share most sections the pressure profiles are very similar.

VA 2: Vacuum technology: New developments and applications

Time: Monday 12:30–13:30 Location: HSZ 301

Invited Talk VA 2.1 Mon 12:30 HSZ 301

Vacuum Solutions for Dilution Refrigerators — •Stefan Lausberg — Atlas Copco - Scientific Vacuum Division, Bonner Str. 498, 50968 Köln

Dilution refrigerators are cryostats that can reach base temperatures as low as 2 mK. The refrigerant they use are mixtures of 3He and 4He that contain about 1/5 of the rare and very expensive 3He. Like in all cryogenic applications, vacuum products play an essential role for dilution refrigerators. In 2019, the world market for dilution refrigerators has increased to more than 200 systems per year driven by the emerging quantum computing market. In consequence, the dilution refrigerator is a growing application for vacuum pumps and accessories like gauges.

Here, we will discuss the requirements for vacuum products in this type of cryostat. Besides pump systems for insulation vacuum and pumps to supply the dilution refrigerator's 1-K-pot, the heart of the cryostat is the 3He pump system. This system circulates the mixture in a closed loop and requires a maximum leak rate of 1E-7 mbar*l/s to preserve the expensive 3He. In order to achieve an enhanced cooling capacity the necessary 3He gas flows require a pumping speed that can only be reached by using a two-stage pump system. We will see that the most appropriate 3He vacuum pump system would be an oil-free, dust-free pump system with an optimized pumping speed in the range of 0.01 to 1 mbar. Even though the pressure range is not within the focus applications of turbomolecular pumps we will see some advantages over roots pumps at the second stage.

VA 2.2 Mon 13:10 HSZ 301

Transient modelling of liquid ring vacuum pumps with mercury as working fluid — •Santiago Ochoa — KIT Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

For an application in fusion reactors, liquid ring pumps with mercury as working fluid are foreseen. This kind of pump is simple and robust in its design, but challenging in modelling: Reliable results - needed to design and optimize liquid ring pumps - can only be achieved if the geometry is modelled in full 3D, considering (turbulent) gas- and working fluid flows through the pump with simultaneous heat and mass transfer. This talk presents a modelling approach of liquid ring pumps with water and mercury as working fluid, using the software ANSYS CFX. In a first modelling step, 3D transient two-phase simulations have been performed using air as pumped gas and water as working fluid. Results will be presented for two different mesh resolutions and operating pressures. In a second step, mercury has been used as working fluid. In this case, it was much more difficult running the model and the computational needs were excessive. However, first results will be presented also here and lessons learned will be shown up.

VA 3: Annual General Meeting

Time: Monday 13:30–14:30 Location: HSZ 301

Duration: 60 min.