

New Links Between Basic Research and Applied Energy R&D

-

The Computational Approach

Berlin, WIAS, 8 – 9 November

Summary

The international workshop held at the Weierstrass Institute (WIAS) in Berlin had been planned as a joint action by the two German Ministries responsible for research and energy technology within the framework of the International Energy Agency's Ad-Hoc Group for Science and Energy Technology (AHGSET). The workshop offered a forum for mathematicians and energy researchers for demonstrating examples of the role that applied mathematics can play in energy science and for discussing opportunities and new paths for enhanced cooperation and "bridging the gap" between mathematics and energy engineering.

Results and Recommendations

by Projekträger Jülich (PtJ)

The workshop's programme was designed taking into account the technical "pull" from engineers and the scientific "push" from applied mathematicians. The topics selected, fusion, fuel cells, combustion, day-lighting, recovery of oil and gas, are all found in the IEA energy research programme. Invited speakers included scientists involved in nationally-supported projects, experts from countries involved in AHGSET and from Switzerland. 40 participants attended the two-day workshop.

The presentations gave an excellent overview of the work being carried out by mathematicians in the simulation and modelling of industrial processes, combustion, fuel cells and the exploration and recovery of oil and gas. The progress made in these areas as a result of faster computers and new mathematical methods was most impressive and work in the field of genetics and theoretical physics, as demonstrated, has led to an amazing acceleration in the speed of acquisition of new information. This methodology can be applied to many topics of energy research.

Modelling of processes and applications found in the use of energy has already been developed systematically with various degrees of success. Complicated combustion processes can still only be described approximately by mathematical models. Modelling of the formation of geological structures to predict the occurrence of possible oil and gas reservoirs and to optimise their production by enhanced recovery methods is even more complex and, as a result, predictions are less reliable. However, the modelling of day-lighting systems and solar-concentrating collectors has reached the stage where models can be used to help in the design of pilot plants and experimental systems. Ways and means of providing impetuses to improve the models and use them more effectively in energy research were discussed. The optimism and commitment of the speakers promised that there is still a lot of room for improvement and that, under the right conditions, progress will continue in the future.

Energy research in recent years has increasingly been concentrating on short-term solutions to specific problems in order to bring new technologies onto the market as quickly as possible and at the lowest possible cost. Research strategies and programmes were oriented towards the short to medium term to achieve tangible results which could be used to justify public spending. Financing long-term objectives aimed at se-

curing the nation's supply of energy for future generations and basic research which could lead to the development of new and innovative approaches to energy research is less easy to justify, particularly in times when the R&D budget is low.

Science mining – the comprehensive screening of results from all branches of basic science for possible applications in energy research – as proposed at recent IEA meetings in Paris was not considered to be an efficient tool for generating progress in energy R&D or defining funding priorities – being too time consuming and expensive. A more strategic approach, bringing together the relevant players and creating an environment conducive to the exchange of knowledge and experience is seen as a more cost-effective solution.

During the workshop it became quite clear that there must be a bridge between basic science - the scientific resources at the disposal of mathematicians - and the problems posed in future energy research. Both energy researchers and mathematicians agreed that the workshop had made an important first step towards building this bridge, and that future activities would be needed. The bridge should, if possible, be planned as an inherent part of future projects at an early stage. However, a precondition for being able to strengthen the bridge and to build on it was seen to lie in the engineer's ability to formulate the problems which the mathematician would then try to solve. On the other hand, new results and processes developed by mathematicians must be made available, in an understandable form, to the engineers and physicists. Clearly even among the mathematicians there is a need for an enhanced exchange of information, particularly in the way in which different problems from applied science are being solved by different groups of mathematicians.

Therefore, it was suggested that a group of highly qualified mathematicians, who are not specialists in any one of the mathematical disciplines (deterministic, stochastic modelling, object-oriented programming, etc.) should form a steering committee to discuss the mathematical approaches to energy-technology related problems. This group would be qualified to evaluate the individual mathematical methods used for the different applications and to make recommendations when new modelling problems arise in the future.

Workshop Presentations: Highlights

by Projektträger Jülich (PtJ)

As part of the AHGSET's strategy to improve the linkage of basic science to energy research, the workshop aimed to identify possible topics where an intensification of contact between mathematicians, representing the science side, and energy engineers would be beneficial. Accordingly, it was a forum for the demonstration of modelling results already achieved and also for discussing the limits of current computational activities. In some cases examples of promising approaches pursued by scientific institutions were presented.

Keynote address: Basic Science and Energy Research

The keynote address was dedicated to pointing out the necessity for a further understanding of material properties by considering recent developments in superconductor research, where applications are running the risk of stagnating due to a lack of understanding of physical phenomena, as well as considering investigations on silicon materials for solar applications. Due to the complexity of these types of research subjects, the need for long-term concepts for materials research and support for comprehensive computer modelling and simulation efforts was emphasised. Bridging the gap between basic research and technology was described as a two-step process, based on three pillars consisting of curiosity-driven research for answering basic questions, applied research aimed at solving problems of high-technology risks, and industrial research striving to develop commercial products.

Introduction: Technical Pull and Science Push

Two presentations discussing the technical pull and the science push from a general point of view reflected the ambiguity of the workshop's subject. Referring to the industrial end-use sector where energy savings are limited due to the dictates of economic conditions, low replacement rates, complex and individually nested process modes, questions of future developments resemble optimisation problems with multi-criteria and multi-objective natures. An analogy to the fundamental processes of basic physical and chemical issues was pointed out. As an example the mathematical approaches based on graph theory and applied to describe the dynamics of particle interactions could be interesting for the treatment of modelling the complex dynamics of industrial processes. A stronger cross-fertilisation between energy technology and related sciences would be beneficial.

From the mathematical perspective, problems arising from energy technologies are usually complex, non-linear, multi-disciplinary and very often beyond the scope of traditional theory. A fundamental tension between the reliability of model results, the complexity of algorithms and implementation performance was observed. From the science point of view, progress on improving the fidelity of simulation and experimental results requires a complete description of problem features to achieve reliable results. Regarding the example of combustion processes, aspects of a multi-physical nature, occurring in multi-scale dimensions have to be considered. Present computer architectures, the data situation and also questions of education and scientific specialisation were identified as barriers to progress. Regarding the development of modelling methodologies, a central role was especially assigned to mathematicians.

Technical Sessions

Session I: Energy Models, Fusion, Fuel Cells, Industrial Processes

Introducing the technologies sessions, two presentations were dedicated to **energy models** as applied by the IEA as well as by individual countries for policy advice. The IEA'S Energy Technology Perspective (ETP) model was developed for the analysis of future energy policies world-wide. It is based on linear programming and a matrix of approximately 5 million non-zero elements. Regarding the role of innovative techniques for future energy simulations it would be very interesting to integrate so-called 'learning-curves' for those technologies. However, present algorithms would be unacceptably inflated by such a procedure. Further measures to improve the quality of energy modelling results would be the coupling of multi-regional models with environmental or economic equilibrium and/or theoretical game models, whereas this would require the availability of faster solvers and improved sensitivity analyses.

In the field of **nuclear fusion reactors**, macroscopic plasma deformations, turbulent transport phenomena and plasma-wall interactions are the subject of comprehensive computation activities. Due to the excellent integration of fusion research teams into the scientific community, the interaction between various disciplines such as physics, mathematics and engineering was pointed out as an outstanding example.

An excellent example of the complementarity of modelling activities as carried out by engineers and physicists as well as by mathematicians was presented for fuel cells. Transport phenomena and chemical interactions occurring in a 2 kW_{th} **solid oxide fuel cell stack (SOFC)** were analysed for various operation conditions by numerical modelling. Striving to optimise the cell and stack performances, the consideration of repetitive processes on multiple scales from micro- to macro-length permits useful approximations. The work shows that ab initio no single method seems to be able to cope simultaneously with all stack issues such as chemical processes, heat transfer and turbulent processes as well as electrical charge transfers. A volume average method and a finite element implementation seem to produce rather promising results. However, a need for better theoretical understanding was noted. The mathematical point of view focussed on the modelling of processes occurring in **direct methanol fuel cells (DMFC)** showing that it seems to be possible to combine modelling of chemical and electrochemical processes with a consideration of energy and heat balances. The comparison of measured data with simulated results showed good agreement, even under various chemical conditions including undesirable parasitic reactions. Improved understanding of elementary processes in the field of catalysts, membranes and also heat transport phenomena would be helpful for the development of materials and components for specific DMFC purposes.

Industrial processes are usually subject to strong technical and economic requirements as well as to the maintenance of quality standards. **Naphtha cracking** for the industrial production of alkenes is a high-temperature and therefore a high-energy-consuming process. A better understanding and control of the formation of coke and related side products was stressed as a key issue for the energetic optimisation of industrial production facilities. Computer modelling would be beneficial to improve the knowledge of carburisation and cracking reactions, of interactions between chemical components and the containment as well as optimisation of the process control.

Session II: Combustion, Conversion, Heat Storage

Combustion and energy-converting processes are traditional fields of close interaction between computational modelling, experimental investigation and engineering activities. Various presentations were dedicated to showing different approaches, applications of scientific work and state of the art of modelling and mathematics.

The session was opened by a presentation on the complexity of **fluidised bed conversion** reactors, where the co-existence of multiphase flows as well as various chemical reactions leads to sophisticated mathematical descriptions. Different time scales of chemical (short) and physical (long) reactions generate additional difficulties for the modelling of the entire conversion process. Aiming at the prediction of ash deposition, the opportunities but also the limits of computational fluid dynamic models were demonstrated. Additional considerations focussing on the reactions in a single bubble showed that a better understanding of the full chemistry, the heat transfer and the treatment of two-phase flows is required.

The importance of high-quality flow models for applications in energy research was highlighted in a presentation showing the results of a collaboration project on **turbulent flows with strong streamline curvature**. Due to insensitivities to rotation and streamline curvatures, classical approaches for flow modelling turn out to be inadequate. Reynolds averaged Navier-Stokes equations (RANS) and large-eddy simulation (LES) permit a fundamental improvement. Additionally, analytical methods based on symmetries (Lie groups) are envisaged to provide essential progress for technical turbulence models. It was pointed out that a comparison of modelled and experimentally produced data verifies the tendency to better simulation results. However, simple models with good prediction capabilities and lower costs are still required.

Quite different approaches are being used in the end use sector, e.g. in buildings, where modelling capabilities and software design is user-dependent and economic aspects require strong links to practice, thus needing to involve customers, architects, designers and others. A presentation on the daylighting simulation system ADELIN which was developed in the IEA Solar Heating and Cooling project showed how the energy load of a building can be reduced by modelling its illumination using various models and algorithms. Integrating complex fenestration systems and models for user behaviour and acceptance are current research topics which could greatly benefit from improved mathematical solutions for the simulation and modelling process.

The sensitivity of the model towards variations of parameters and the reliability of model results are important for the quality and usefulness of computational work. In most cases, sources of uncertainties or errors in modelling descriptions are caused by uncertainties of the model itself, of the parameterisation or of the numerical discretisation. Stochastic measures offer a useful method for the quantification of these uncertainties and, furthermore, they enable a judgement to be made on the efficacy of the model analysis. A basic research application for these uncertainty analyses was presented showing as an example the impact of fast changes in chemical reactions occurring in combustion processes including ignition processes and regions

of explosive mode growth producing instabilities. **Stochastic uncertainty quantification techniques** offer significant analysis capabilities for the description of these processes. A further approach to cope with the growing demand for computation time relating to a better understanding of combustion processes and flame reactions was presented by highlighting the expected further evolution of future computer generations. Based on a consideration reflecting the past development of storage capacities and their exponential growth, the predicted computation capacity will permit appropriate calculations of complex algorithms within a few decades.

Turbulent flows are not only of interest for combustion processes, but also play a central role for some renewable technologies such as **wind turbines**, where turbulent wind flows and the aerodynamic behaviour of the turbines are important subjects of modelling activities. Current practice shows that interactions between wake and rotor are complicated and characterised by non-linearities. Due to the small time scales of steady conditions, the simulation, especially of large turbines, requires high temporal and spatial resolutions with consequently long calculation times. The application of Navier-Stokes studies and RANS as well as LES models was recommended, although further improvement of the physical understanding of the machines' performances and the need for experimental validation of modelling results were emphasised.

The modelling of energy systems could address very different fields of physical and chemical relationships. An interesting option for the convenient creation of a simulation tool addressing all the basic physical reactions is offered by the Modelica instrumentation, based on an **object-oriented simulation approach**. Clearly designed standard components, provided by various Modelica libraries, could be combined based on differential, algebraic and discrete equations. The easy and convincing application of Modelica for heat storage facilities was demonstrated.

Session III: Energy and Geology

The role that geological modelling, flow simulation and reservoir modelling can play in the forecast of **oil and gas reservoir production** and the interlinkage between short and long-term technology needs for geology and recovery processes in the **oil and gas** sector were the subjects of the next two presentations. Basin and stratigraphic modelling of sedimentary basins is a complex process which is being combined with geological models, 4D seismic and well data and with hydrocarbon reservoir modelling to forecast production data and to assess their uncertainties. Simulation of the behaviour of oil and gas flows using refined grids in reservoir zones and applying the equations of fluid flow dynamics at the given or estimated petrophysical properties requires adequate mathematical approaches, efficient modelling methodology and high computer power. With new approaches applying improved mathematics for the modelling processes, better and more reliable results could be achieved. The presentation demonstrated the possibilities of advanced models, comprising extensive visualisation options striving to assist the understanding of complicated relations.

The interlinkage between short- and long-term technology needs within geology and recovery processes in the **oil and gas** sector was the subject of two presentations. Modelling the behaviour of petrophysical properties by the application of basin models and fluid flow dynamics enabled new results on geological environments to be achieved. A presentation was given on the possibilities of advanced models, comprising extensive visualisation options to assist the understanding of complicated relations. In a second contribution, referring to Norwegian oil production, emphasis was given to the extraordinary role which public research can play even in an area which is dominated to a large extent by commercial interests. Present collaboration activities such as the IEA's Implementing Agreement on enhanced oil recovery were presented as suitable tools for gathering international expertise from industry as well as from the scientific communities. It was, however, noted that future requirements in the field of oil and gas exploration will rely on sufficient competence, expertise and new ideas arising from basic research.

The **storage of CO₂** in underground reservoirs is of increasing interest for fossil-fuel-dominated energy systems. The simulation of the behaviour of stored carbon dioxide in former gas fields including sedimentation aspects or the spreading of the gas in Bunter sandstones showed remarkable results. It was concluded that the availability of appropriate modelling instruments is satisfactory, although the coupling of various aspects such as geochemistry, fluid dynamics and economic considerations leaves room for improvement. Furthermore, the need for models for long-term predictions as well as experimental verification of numerical results was also mentioned in this context.

Session IV: Mathematical Outlook

The workshop was completed by a mathematical presentation describing options offered by **genetic programming**, based on algorithms similar to the behaviour of a set of individuals in a population and their development. The relevance of this approach for many aspects of the oil and gas sector was pointed out.

Present and Future Role of Applied Mathematics and Scientific Computing

by Weierstrass Institute for Applied Analysis and Stochastics (WIAS)

The mathematical problems discussed during the lectures focused on fields which have for many years been under intensive study by researchers from applied mathematics and from scientific computing: materials science, combustion, computational fluid dynamics (CFD), reaction-diffusion-convection problems, magneto-hydrodynamics. While in CFD scientific computing is a commonly used tool, there are other fields in which the expertise of modern applied mathematics and scientific computing is still not fully employed or is even unknown.

Some of the problems, which occur for instance in reactive flows and combustion processes, will not be accessible to a direct mathematical treatment even in the nearer future. On the other hand, the successful treatment of cases with reduced kinetics, simple geometries, moderate velocities, and mainly local interactions, will be possible.

To this end, it seems to be indispensable to make intelligent use of modern techniques from the fields of applied mathematics and scientific computing. In this connection it is very important to realize from the very beginning that it would be completely erroneous to believe that it will suffice just to buy faster and larger computers.

An approach which is solely based on an increase of the available computer power will eventually fail !

Instead, it will be absolutely necessary to recur to the whole chain of mathematical modelling, from analysis, the construction of numerical techniques, the generation of appropriate discretization grids, the development of optimal algorithms, to, eventually, the production of fast and reliable simulation software.

In order that the incorporation of mathematical expertise be successful, it is absolutely necessary to increase the scientific exchange between mathematicians, physicists, engineers, and also economists working in the field. The problems to be solved are obviously interdisciplinary, and thus can only be solved by a joint effort of the different disciplines.

In Germany, such interdisciplinary working groups involving applied mathematicians exist in many areas. With regards to energy sciences, a main field of such activities is the modelling of fuel cells. In this area, mathematical groups at the universities of Freiburg and Bayreuth, as well as at the Weierstrass Institute (WIAS) in Berlin, cooperate with experts from the applied sciences, supplying mathematical models and high quality software tools for the numerical simulation of realistic configurations.

Organisation of Future Research

During the workshop it became very evident that in many cases the interaction between basic and applied research is insufficient and/or inefficient, and the necessary interdisciplinary research (also between the different fields of energy science) is obviously not the rule. This will have to be changed fast.

As explained above, a successful incorporation of the tools of modern applied analysis and scientific computing in the solution process makes the formation of interdisciplinary working groups necessary. This however, will only be possible for selected types of problems and not in all situations. It would make sense to define energy technologies, (finite) time horizons, and key problems having a certain universality and expected lifetime, in which interdisciplinary efforts should be concentrated. We therefore advise the funding agencies **to concentrate both organisation and funding on selected key technologies in energy research.**

In this way, exemplary scientific and industrial projects could be brought to a solution in a reasonable time, and the exchange between basic sciences and applied industrial research could be improved. At the same time, applied mathematicians have a request to the funding agencies that also applies to other fields, not only to energy research:

If in a proposal for a publicly funded research project funds for numerical simulations are applied for, then the applicants should provide evidence that the numerical techniques they want to use meet the standards of modern applied mathematics and scientific computing.

Otherwise, there is a big danger that expensive computer time and manpower will be wasted for non-optimal and unreliable software solutions.