# THERMODYNAMICS OF NUCLEAR MATERIALS

An important group of problems concerning the materials used in nuclear technology was discussed at a Symposium on the Thermodynamics of Nuclear Materials, held by IAEA in Vienna from 21 - 25 May 1962.

In general, thermodynamics is the study of laws governing processes which involve heat changes. It includes the study of conditions under which various substances exist in chemical equilibria, the consequences of chemical reactions and the interchange of heat and other forms of energy when a chemical reaction occurs. In the field of nuclear technology, it is necessary to know how construction materials melt or evaporate, the solubility of fuels, the chances of chemical reactions between various materials used, and the energy of reaction if a reaction takes place. Together with the study of certain other properties of nuclear materials, thermodynamics provides one of the fundamental guides in modern nuclear technology, especially in the development of high-temperature reactors and of new methods for the reprocessing of spent fuels.

Opening the symposium, Dr. Sigvard Eklund, Director General of IAEA, said that during the development of nuclear technology, especially during the last few years when more and more emphasis had been put upon the development of high-temperature reactors, the properties of nuclear materials had become a subject of increasingly greater interest. Obviously, said Dr. Eklund, this interest stemmed from an effort to achieve higher efficiency in reactor performance, greater reliability and longer reactor life. And it was equally obvious that all these characteristics had a direct bearing on the prospects of making atomic energy an economic source of power.

Dr. Eklund pointed out that the thermodynamic problems of nuclear materials could be investigated not only in atomic research centres, but also at other scientific institutes, and research in thermodynamics had, in fact, been carried out at a number of different laboratories treating different elements, compounds and systems. Contributions to this subject in recent years had been so large and widespread that it had been considered useful to organize a meeting at which scientists from different countries could discuss the present status of research on the thermodynamics of nuclear materials.

### **Topics of Discussion**

The first session of the symposium discussed in general the thermodynamic properties of actinides, i.e. the elements starting from actinium upwards in the Periodic Table, including thorium, uranium and plutonium which provide reactor fuel. The second session was devoted to applications of thermodynamic theory to the study of nuclear materials, while the experimental techniques for the determination of thermodynamic data were examined at the next session. The thermodynamic properties of alloys were considered at a separate session, and another session was concerned with solids other than alloys. Vaporization processes, which are of special interest in the development of high-temperature reactors, were discussed at a separate session.

Since the symposium was attended by both scientists who produce thermodynamic data and technologists who apply these data to practical tasks, the discussions on the methods of developing the data and ascertaining their accuracy were especially useful in highlighting the importance of determining whether any given data are reliable before they can be put to practical application. In fact, thermodynamic data have often been applied to practical problems of engineering and technology without due consideration of their reliability, and an important outcome of the meeting was to emphasize that since thermodynamic properties are basically related to other physicochemical properties, no dependable thermodynamic data could be derived without full investigation and understanding of the chemical composition of the various phases of a material. If the chemical composition of the different phases is relatively simple (such as  $X/solid/\rightarrow X/gas/$ ), the thermodynamic properties can be deduced in a fairly straightforward manner. But if the chemical species involved in a particular reaction is not clearly known (as is often the case in the gaseous phase), the derivation of thermodynamic data can only be based on untested assumptions.

Many alloys and refractory materials (i. e. materials which evaporate only at very high temperatures) are of great importance in nuclear technology, and some of these substances are extremely complex in their chemical composition. For example, until recently the phase composition of the oxides of thorium, uranium and plutonium had been only very imperfectly understood, and the same was true of the carbides of these elements.

Recent developments in experimental techniques have made it possible to investigate the phase composition of these complex materials as well as the chemical species of these materials in the gaseous phase. For example, mass spectroscopy has considerably helped in determining the gaseous species of refractory materials. As a result, it has now been possible accurately to determine the thermodynamic properties of such materials, and a considerable volume of data has already been accumulated. Simultaneously, recent developments in measuring techniques, such as fluorine bomb calorimetry and Knudsen effusion technique, have greatly increased the accuracy of thermodynamic data.

### Accomplishments and Tasks

The discussions at the Vienna symposium showed that the determination of the thermodynamic properties of uranium oxides with the help of the newly developed experimental and measuring techniques had been largely accomplished, but there was still a great deal of work to be done on carbides. The data on uranium carbides presented at the symposium showed that different values had been obtained at different laboratories and intensive further investigation was necessary to resolve these differences.

Considerable interest was evinced in the vaporization processes of nuclear materials, especially because of their bearing on the development of hightemperature reactors. Besides, there was an extensive discussion on how the principles of thermodynamics could be applied to practical problems in nuclear technology. For example, it was shown how the composition of alloys, which are often used as reactor materials, could be theoretically predicted from thermodynamic data. Development of this method would obviously save a great deal of experimental effort on the part of metallurgists.

At an informal session of the symposium, the participants discussed in general the need for a critical evaluation and compilation of thermodynamic data on important nuclear materials. It was apparent that in view of the increasing volume of data being developed through research in thermodynamics at various centres, there was a growing need for the pooling and comparison of these data and for the dissemination of the evaluated results for use in nuclear technology throughout the world.

The following scientists presided over the individual sessions of the symposium: C. W. Beckett (USA), O. Kubaschewski (UK), T. Mukaibo (Japan), H. Nowotny (Austria), F. Reshetnikov (USSR), S. Varsano (Italy), R. F. Walker (International Union of Pure and Applied Chemistry), and F. E. Wittig (Federal Republic of Germany). The informal session was presided over by K. Schäfer, Chairman of the Commission on Thermodynamics and Thermochemistry of the International Union of Pure and Applied Chemistry.

# ANNUAL REPORT TO ECOSOC

The development of the work of the International Atomic Energy Agency during the past year is outlined in the Agency's latest annual report to the Economic and Social Council of the United Nations (ECOSOC). The report covers the period 1 April 1961 to 31 March 1962.

The report gives an account of scientific and technical work in the three principal fields of interest to the Agency, namely (i) nuclear power, reactors, fuels and materials, (ii) radioisotopes and radiation, and (iii) protection against radiation. The programmes and activities are then summarized in three sections representing the three principal forms of the Agency's operations, namely (i) technical assistance, (ii) exchange of information, and (iii) research and development. Some of the main points of the report are reproduced in this article.

#### Nuclear Power, Reactors and Fuels

Member States have shown increasing interest in the possibilities of undertaking nuclear power projects with the Agency's help. In June 1961, an Agency mission made a preliminary survey of the possibility of establishing a demonstration power reactor in Yugoslavia, which might be designed, built and operated as an international enterprise. The mission's preliminary assessment of the technical aspects of the project was favourable. Another mission visited Pakistan in January this year to evaluate the prospects of nuclear power in that country and to review a study of the subject made by the Pakistan Atomic Energy Commission and its engineering consultants. (The findings of this mission are reported in a separate article in this issue of the Bulletin.) The report of an earlier mission, which studied the prospects of nuclear power in the Philippines, was published during the year. (See Bulletin Vol. 3, No. 4.)

A number of Member States have indicated difficulties in making full use of research reactors that have recently come into operation or are now under construction. A major difficulty is the lack of adequate scientific and technical personnel to make full use of the reactors, operate them safely, and plan programmes for reactor experiments. The Agency is trying to help overcome such difficulties through its training and technical assistance programme, and by organizing scientific meetings on the problems involved.