IGC newsletter

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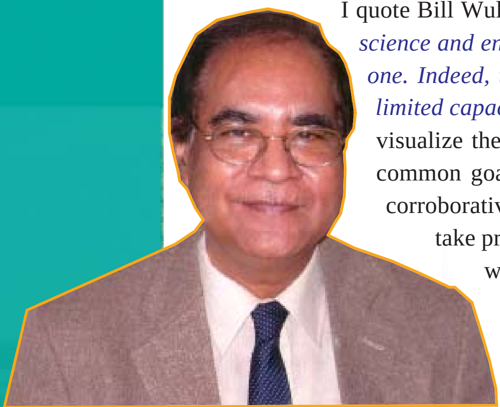
From the Director's Desk

NEW YEAR MESSAGE

It gives me a great pleasure in wishing you and your families a very happy and blissful New Year and a Happy Pongal.

The Centre visualizes world leadership in Fast Reactor and associated Closed Fuel Cycle through robust and safe technologies based on breakthroughs provided by basic science and engineering disciplines. I am a firm believer in seamless science and technology. I quote Bill Wulff *"There is only one nature - the division into science and engineering is a human imposition, not a natural one. Indeed, the division is a human failure; it reflects our limited capacity to comprehend the whole"*. We thus have to visualize the totality of the picture and evolve towards the common goal of the Centre, with our complementary and corroborative contributions relating to our specializations. I take pride in sharing a few achievements of the Centre with you.



The Fast Breeder Test Reactor (FBTR), the pride of the Centre, has continued to scale new international heights by successfully operating and making the mixed carbide fuel reach a burn-up of 155 GWd/t, without any fuel failure. FBTR is also acting as a test-bed for the PFBR MOX fuel, which has already undergone 60 GWd/t of burn-up as against target burn-up of 100 GWd/t. This will provide very valuable data on the irradiation behavior of the oxide fuel. We have received regulatory clearances for doing some state-of-art and relevant experiments to enhance safety of future Sodium Cooled Fast Reactors. Analytical and experimental investigations are being pursued towards life management of FBTR to ensure that FBTR is available to us for next twenty years.

The Prototype Fast Breeder Reactor (PFBR) construction has progressed as scheduled, and we are sparing no efforts to ensure that it will be commissioned by September 2010. The Centre continues to provide robust design and R & D support to PFBR. A

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few important components like Safety Vessel, Main Vessel and Inner Vessel have arrived at site. Many of the reactor components are in advanced stage of fabrication. It is a matter of great satisfaction for us that we have achieved quality levels better than specified and also many international benchmarks.

Closing the fuel cycle is very important and critical aspect of Fast Reactor technology and thus reprocessing of the spent fuel is very crucial for this. We are taking all necessary and urgent steps towards robust fuel cycle technologies. Integrated Fast Reactor Fuel Cycle Facility (FRFCF) co-located with Prototype Fast Breeder Reactor (500 MW(e)) is making good progress. Work on plant design engineering consultancy has been completed, including the geo-technical work, which is important aspect of the plant safety. Activities connected with the Head End Facility are in progress to integrate with Demonstration Fuel Reprocessing Plant (DFRP) to be commissioned in 2009. DFRP is designed for reprocessing irradiated FBTR fuel on regular basis and demonstrating 'process and plant' for reprocessing of irradiated mixed oxide fuel of PFBR.

The full power operation of the Steam Water System of the Steam Generator Test Facility (SGTF) is an event that we are keenly looking forward to. The operation of the SGTF would provide valuable insights into the design and operation of the steam generators, which are vital for FBRs. Similarly, the testing of various components in sodium and the setting up of the full scale simulator for PFBR are in exciting periods of progress.

While we note with pride our Centre's progress so far, we realize the need to embark on an intense and focused long term R&D programme to introduce innovations in reactor design, construction and operation as well as the fuel cycle so that the reactors and the fuel cycle facilities not only provide power at an economical tariff but also operate safely with high availability factors. Our Centre has already arrived at a framework of R&D programme, which has to be pursued in order to meet these objectives The R&D programmes encompass many areas of science and technology including physics, chemistry, structural mechanics, electronics, safety etc. Thus it is obvious that the entire Centre must focus on these R&D programmes in order to elevate the fast reactor programme to higher domain. It is very important that we involve all the young minds of the Centre to ponder over the issues related to economics and safety of the reactors and fuel cycle and take up R&D programmes with commitment and focus.

We have a unique opportunity to play a leading role in the global development of fast reactors and fuel cycle. It is not an exaggeration to state that our success in the PFBR project and associated closed fuel cycle will be an important ingredient, in subsequent decisions about the development of fast reactors and their enhanced contribution to nuclear energy production not only in our country, but also other countries. The world nuclear community is watching with keen interest and admiration our progress in fast reactor technology. We must make every effort to achieve total success in these programmes and also keep up the momentum of R&D to reach higher levels of maturity in this technology.

We have always believed that quantum jumps in technology can only take place through scientific breakthroughs. It is for this reason that we have a strong and focused programme of basic research in our Centre, covering a wide spectrum of activities such as ab-initio computations, nano coatings, etc. To further strengthen our human resources and the vitality of our Centre and continuity of knowledge, we have started a Training school at IGCAR in core engineering disciplines starting from this year. While, presently it caters to chemical engineering, electronics and instrumentation and mechanical engineering, we hope to add more disciplines in the years to come. With IGCAR becoming a constituent institution (CI) under Homi Bhabha National Institute (HBNI), having a university status under University Grants Commission, we can hope to further strengthen our human resources by inducting more young students in various research programmes, besides fulfilling the academic aspirations of our colleagues. This definitely provides a rich academic atmosphere to our mission-mode research programmes.

While providing the impetus to the R & D activities at IGCAR through careful planning and focused execution, we have also kept in mind the improvements in the residential environment and holistic health care for the residents. Construction of protection wall for the Township has been completed and the construction of another bridge for the township is in progress. The schools on their part have continued to provide the right environment for nurturing excellence in students. All these augur well for the overall comfort, safety and blissful living of our colleagues.

Fast Reactor Science & Technology is an important area, where continuous quest for knowledge, understanding and innovations is necessary to enable a quantum leap in our endeavor to be a world leader. We should evolve and mature from the questions of *"What ? Why? How ?"* to aiming for bigger things and be confident to ask *"Why not ?"*. Let me quote Albert Einstein, *"The mere formulation of a problem is far more essential than its solution, which may be merely a matter of mathematical or experimental skills. To raise new questions, new possibilities, to regard old problems from a new angle require creative imagination and marks real advances in science."* Let us all march together to attain such a state of collective scientific maturity and wisdom.

Wish you and your family all the bliss, happiness and prosperity during the year 2007.

(Baldev Raj)
Director
IGCAR & GSO

Aerosol Test Facility for Fast Reactor Safety Studies

During normal operation of a nuclear reactor, there is a balance between the heat generated in the core and the heat removed by the heat exchanger. If the heat removal is less than the heat generation, the excess heat will be dissipated in the core itself. The cause of this excess heat may be due to the following more probable initiating events in the reactor: (i) Transient over power initiated by reactivity addition (TOP), (ii) Loss of coolant initiated by reduction in the flow of coolant liquid (LOF), and (iii) Loss of coolant initiated by loss of heat sink (LOHS). The development of these initiating events are detected, and by taking suitable action, the reactor is brought to normal condition within a safe period of time. Any failure in detection and prevention measures may lead Core disassembly, Core melt-down or both. The after effects of core disruptive events are called core disruptive accidents (CDA). In order to prevent the initiating events of CDA, the following two safety systems are provided in the reactors: (i) Shut Down System (SDS) and (ii) Decay Heat Removal System (DHRS). The above systems are normally designed to have the failure probability better than the mandatory requirements of 10^{-6} / reactor year for SDS and 10^{-7} / reactor year for DHRS. Therefore, in case of initiating transient event occurring in the nuclear reactor, the CDA can be expected only when the above two safety systems fail. In other words CDA is viewed as the consequence of the initiation events followed by the failure of SDS and DHRS.

In the case of most unlikely event of Core Disruptive Accident (CDA) in Liquid Metal Fast Breeder Reactor (LMFBR), the sodium slug may impact the reactor vessel head, causing damage. This provides a pathway for the escape of radioactive material (fission products and fuel material) and sodium into the containment. Fuel and fission product vapors will condense and form aerosols. In addition, sodium burning will give rise to various compounds of sodium aerosols. In the bottled condition of containment, it is expected that only gaseous and aerosol materials may leak through the containment building to the environment. The leak will be mainly through the ducts and wall penetrations. The amount and type of aerosol released depends on the following two factors: (i) the concentration of the aerosols inside the containment at various times following the postulated accident and (ii) the leakage rates from the containment stack, ducts and cracks. The time evolution properties of aerosol mass concentration inside the containment building and aerosol material deposition on the walls and floor of the containment building are also of great importance. Knowledge of these properties is required for the analysis of corrosion of building material and equipments and also for the planning of the subsequent cleaning and calculating the sodium aerosol exposure for the operating personal. For the post accident management of fast reactor, the use of validated computer code such as HAARM code is needed. The computer code predicts the following characteristics: (i) the behavior of sodium, fuel and fission product aerosols inside PFBR containment and (ii) the subsequent transport into the atmosphere.

In sodium cooled fast reactor, aerosols are generated in the case of sodium leak from the secondary loop, apart from the CDA case. The hot circulating sodium in the secondary loop may get in contact with atmosphere through cracks and burns

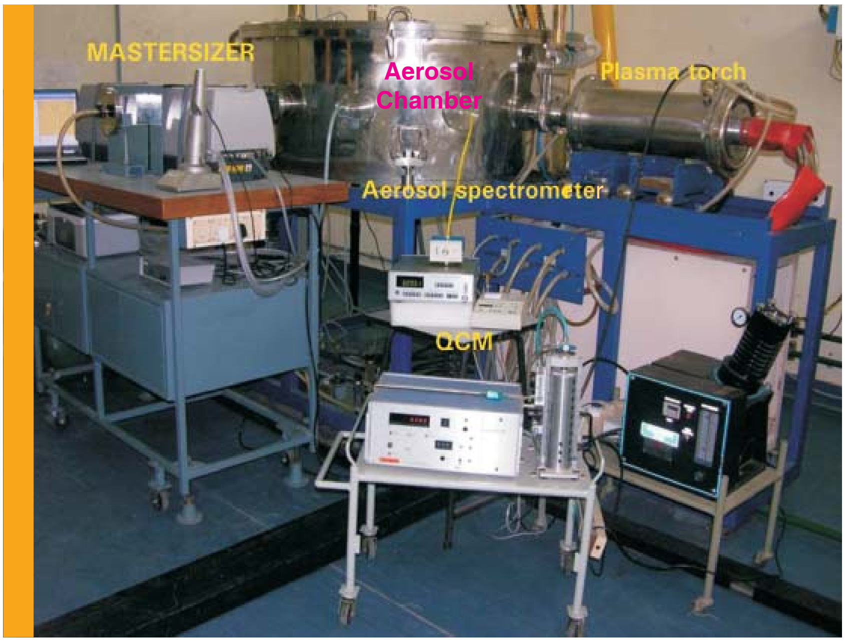


Fig.1 Photograph of Aerosol Test Facility showing plasma torch, aerosol chamber and aerosol diagnostic equipments.

to give aerosols. In atmosphere, hot sodium burns to give sodium monoxide (Na_2O) when sodium is in excess and peroxide (Na_2O_2) when oxygen is in excess. The oxide aerosols quickly react with water vapor present in the atmosphere forming sodium hydroxide (NaOH) and then sodium carbonate (Na_2CO_3) upon further reaction with carbon dioxide in the atmosphere. Sodium compound aerosol is a mixture of all the above compositions and the proportion depends on oxygen, atmospheric moisture and CO_2.

For the aerosol studies of fast reactor safety analysis, an Aerosol Test Facility (ATF) has been designed fabricated and Commisioned at Radiological Safety Division (RSD). The test facility is used for the generation of input data for HAARM code and for the studies on co-agglomeration processes of the mixture of sodium, fuel and fission product aerosols. The aerosols of sodium, fuel and fission product will be generated with the requisite mass concentration and the aerosol studies are being carried out. The materials used for the generation of aerosols are of non-radioactive fission products such as strontium peroxide (SrO_2), barium oxide (BaO) and cerium (IV) oxide (CeO_2) and coolant sodium. A photograph of ATF facility is shown in Fig 1. ATF mainly consists of an aerosol chamber, a plasma torch for the production of aerosols of fission products and fuel equivalent materials, a sodium combustion cell for the production of sodium oxide aerosols, aerosol measurement apparatus, humidity controller and auxiliary systems such as water cooling, air flow, gas flow, pneumatic control, vacuum, material handling systems and on-line data acquisition system for temperature, pressure and relative humidity (RH) during experiments.

Aerosol Generation

A 25 kW thermal plasma torch is operated in non-transferred arc mode. Plasma torch is based on arc ignition between a thermionic tungsten cathode and a co-axial copper anode, both of which are water-cooled and immersed in an axial magnetic field. Nitrogen is used as the plasmagen gas. Nitrogen or argon can be used as the sheath gas. Two methods are employed in this system for the production of aerosol viz., powder feeder and wire feeder. The powder feeder is an instrument to introduce the powder into the flame at the required rate. The wire feeder has a stepper motor driving system, where the wire or a tube of 6mm diameter, can be fed into the flame at the required rate. The material introduced in the plasma flame is ensured with higher dwell time. During the time, the high enthalpy available in plasma is utilized to dissociate, melt and/or evaporate finely divided particles introduced into the flame to produce dispersed aerosols by evaporation-condensation process.

Sodium combustion cell is used for the generation of sodium compound aerosols. A Bunsen burner (capacity ~ 150 gm) is kept inside a vacuum compatible chamber. An external heater energizes the burner. The temperatures of the sodium and at locations just above the sodium are monitored using thermocouples. The sodium combustion cell is flushed with argon and it is isolated from the aerosol chamber through a pneumatically operated gate valve. Sodium is loaded in the burner and it is heated in argon environment. After heating the sodium to the required temperature (say 550^{o}C), compressed air is passed in to the cell through a valve. The sodium burns and forms into aerosols and the sodium compound aerosols are injected into the aerosol chamber.

Aerosol Characterization

Characterization of aerosols is done by (i) Real-time and (ii) Cumulative samplings. The aerosol deposits are analyzed in SEM, EDAX and XRD analyzer. Using light scattering devices such as Mastersizer (M/s Malvern UK), Aerosol Dust Monitor (M/s Grimm Aerosolteknic, GmbH, Germany) and Quartz Crystal Microbalance (QCM) (M/s California Instrument, Inc., USA), real time measurements are carried out. Filter paper sampler and Low Pressure Impactor (M/s Andersen Inc., USA) are used for cumulative measurements.

Experiments

The initial (at a time t=20s) volume-sized distribution of sodium compound aerosol measured by Mastersizer at 50% Relative Humidity (RH) is shown in Fig.2. The initial sized distribution is a Gaussian log-normal distribution having Mass Median Diameter (MMD) of 1.02 µm with Geometric Standard Deviation (σ_g) (GSD) 1.2. Mass-size distribution was measured by QCM at the instant of 20s and it is also a log-normal distribution with Aerodynamic Mass Median Diameter (AMMD) at 1.58µm with GSD (σ_g) of 2.75. Upon converting AMMD to MMD by using the density (2.2 g/cm^3) of the sodium hydroxide (the nature of the aerosol), the MMD was found to be almost equal to 1.0 µm. The initial MMD was obtained for various ignition temperature of sodium and found to be nearly 1.0 µm. The initial MMD was also determined by various RH% inside the chamber. It was observed that, the initial MMD value is nearly 1.0 µm up to 50% and then it increases with increase in RH value.

The depletion of mass concentration with time inside the closed vessel for the sodium oxide aerosol, SrO_2 and Fe_2O_3 aerosols is shown in Fig 3. The depletion rate of mass concentration of the sodium compound aerosols is

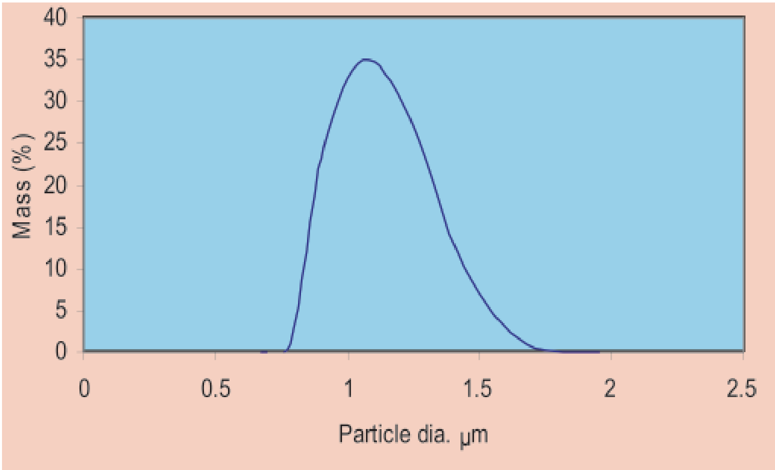


Fig.2 The initial Mass-size distribution (20s) of sodium compound aerosols for the ignition temperature of 550 °C at 50%RH measured by Mastersizer.

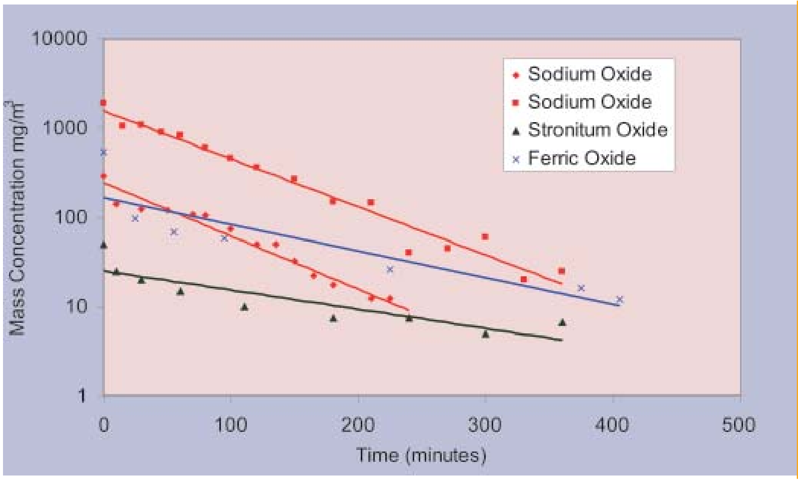


Fig.3 The depletion of mass concentration of sodium compound aerosol along with Fe_2O_3 and SrO_2 aerosols

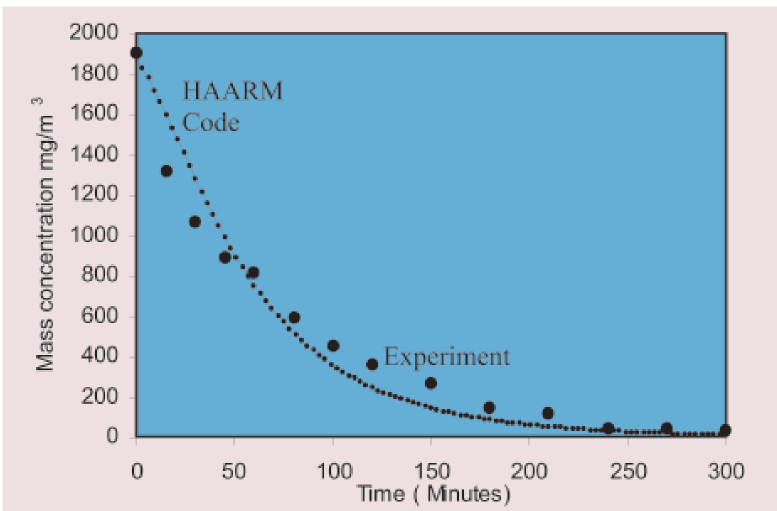


Fig.4: Depletion of suspended sodium compound aerosol mass concentration with time in the absence of gamma field

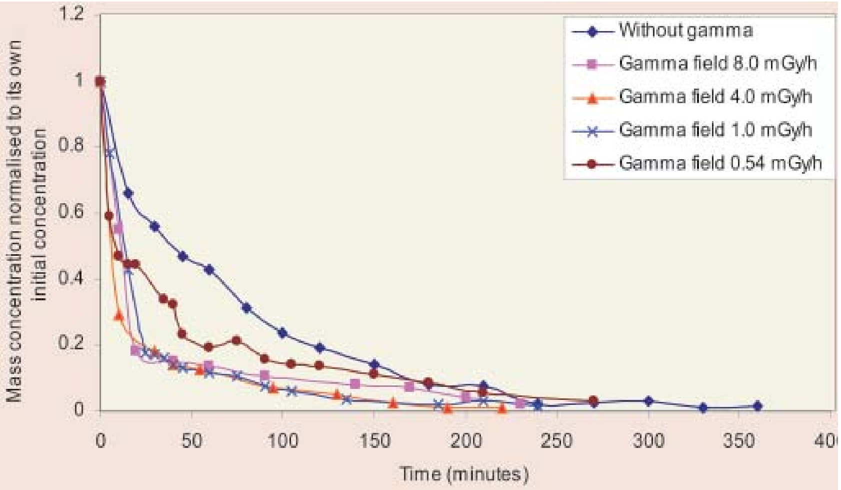


Fig.5: Depletion of suspended sodium compound aerosol mass concentration with time under gamma field

faster than that of SrO_2 and Fe_2O_3 aerosols. This is attributed to the fact that sodium oxide reacts with humidity and size grows, which enhances the coagulation resulting particle size. The larger particles undergo faster gravitional settling. The initial aerosol mass concentration inside the chamber is nearly 2 g/m^3. Using initial MMD and mass concentration as input, the time evolution of suspended mass concentration of the sodium compound aerosols inside the chamber was predicted by HAARM code. Both experimental and HAARM code predictions are presented in Fig. 4.

A ^{137}Cs source of strength 60 GBq was used for the panoramic exposure of the aerosol chamber. The time evolution of suspended aerosol mass concentration (sodium compound) inside the chamber under the gamma field was studied for the dose rates of 8.0, 4.0, 1.0 and 0.5 mGy/h and these results are shown in Fig. 5. It is observed from the Figure 5 that, the aerosol mass concentration decreases faster in the presence of gamma field. The faster depletion rate is attributed to enhanced Brownian coagulation due to bi-polar charging of aerosols.

Summary

Aerosol study is one of the important areas of interest in the fast reactor safety analysis. The environmental source term and consequences of sodium leakage depend on the amount of aerosol released and their characteristics. In this context ATF is used to generate input data for various analyzing codes and predict models in the case of such leakages. Further experiments are being continued with composite aerosols.

(Reported by R. Baskaran, V. Subramaniam and R. Indira Radiological Safety Division, SafetyGroup)

Sensors for monitoring of transformer oil and ethanol mixed petrol as spin-offs from the pulsating sensors development programme

Novel approaches in the development of Sensors for diverse applications at the Centre led to the creation of a variety of pulsating sensors. The in-house developed sensors of unique designs are facilitating development of reliable, inexpensive and high performing real-time instrumentation systems for general as well as for special purpose applications relevant to our reactor and associated fuel cycle programmes. Here we report two spin-off developments which are of wider significance to the energy sector.

I. Transformer oil degradation monitoring

Slow build up of oxidation products as a result of chemical reactions with oxygen and moisture from environment under the prevailing service conditions and physical ingress of polar molecules such as water cause the dielectric permeability of the service oil in any transformer to increase with time. A pulsating sensor has been developed for monitoring transformer oil degradation. The sensor is basically capable of detecting minor shift in dielectric permeability of the oil during service. A laboratory made stainless steel electrode assembly consisting of uniformly spaced multiple number of SS electrode discs, immersed in the mineral oil of interest, serves as the timing capacitor of an oscillator circuit which is driven by a DC supply. With all other factors remaining unchanged, the digital pulse frequency at the output is governed by the dielectric permeability of the oil that acts as the dielectric medium in the capacitor assembly. The pulse frequency changes sensitively with the change in dielectric permeability and, hence, the shift in measured pulse frequency with respect to the fresh oil is a measure of dielectric degradation of the used oil during service.

The measurement set up is shown schematically in **Fig.1**. Frequency can be measured by any of the commercially available hand-held frequency meter. However, for a detailed study hardware and software interfaces have been developed to record the frequency data as a function of time through a PC. Photographs of a typical field monitoring kit and a PC based measurement device, both developed at IGCAR, are shown in **Fig. 2a** and **Fig. 2b** respectively.

The digital pulse frequency data as a function of time for fresh oil as well as for a slightly degraded oil using a typical device is shown in **Fig. 3**. Decrease in pulse frequency for the used oil corresponds to increase in the dielectric permeability by about

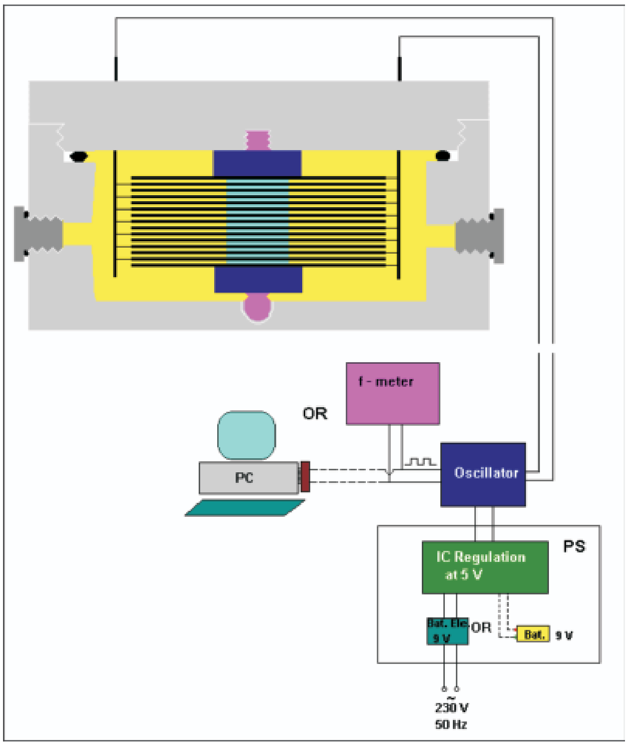


Fig. 1 : Schematic representation of the oil monitoring device.

Fig. 2 : a) A typical pulsating sensor based transformer oil field monitoring kit. b) A PC based data acquisition system for the oil monitoring device.

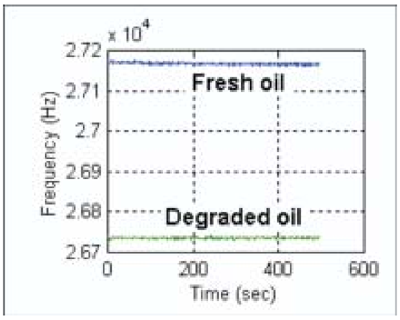


Fig. 3 : Pulse frequencies recorded as a function of time for fresh oil and a sample of service oil.

Fig. 4 : A prototype on-line transformer oil monitoring probe.

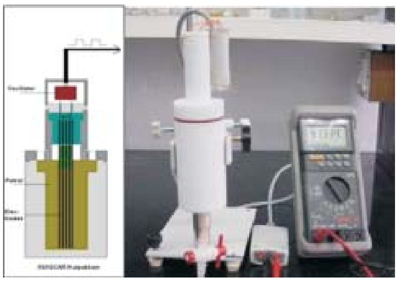


Fig. 5 : The schematic diagram with a photograph of the portable field monitoring kit for assay of ethanol in petrol.

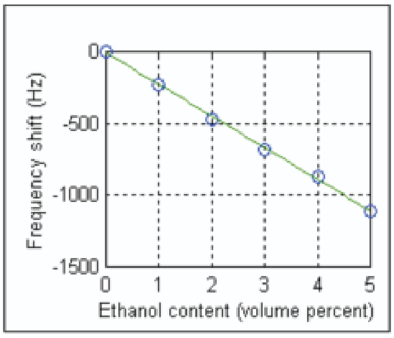


Fig. 6 : Response of the device to ethanol.

1.6 %. Thus, extremely high precision in frequency data permits monitoring of very minute shifts in dielectric permeability, hence enabling early detection of onset and progress of degradation in the quality of service oil.

Under an MoU between IGCAR and Central Power Research Institute (CPRI), the devices made in IIS for ESD of IGCAR were tested at CPRI along with the conventional standard techniques for degradation assessment. Two hundred oil samples from power transformers of different ratings were collected and evaluated by the Dielectric Laboratory of CPRI for the standard characteristics viz., interfacial tension, neutralization value, dielectric dissipation factor, resistivity, breakdown voltage and water content following the prescribed procedures. The digital pulse frequencies were also recorded by CPRI on each sample using the pulsating sensor based oil monitoring devices. Thus, seven parameters were determined experimentally on every oil sample.

It was observed that the pulse frequency, as measured by the IGCAR devices, reduced by about seven percent for service oils nearing rejection compared to that for the fresh oil. As the devices permit precise measurement of frequency shifts less than 0.2%, onset of degradation is detectable at an early stage. Further, the correlations among the standard characteristics, ie among interfacial tension, neutralization value, dielectric dissipation factor, resistivity, breakdown voltage and water content, were comparable with those between the digital pulse frequency and the standard parameters. The conclusion of the joint evaluation by IIS, ESD and CPRI was that, as the pulsating sensor based new technique of IGCAR is simple, the transformer maintenance personnel may use it as a screening test for deciding whether the oil sample should be sent to a central laboratory for full evaluation towards further actions with respect to treatments for reuse or disposal.

Success of the off-line devices prompted design and development of the rugged on-line monitoring devices at IIS in collaboration with ESD. Photograph of an on-line prototype device which is in operation for over one year with an 11-kV transformer in IGCAR is shown in **Fig. 4.** Industrial grade products have also been made and they are undergoing laboratory tests.

II. Ethanol assay in ethanol mixed petrol

The laboratory developed digital approach, enabling capture of minor variations in dielectric permeability of liquid dielectrics, led to development of a portable battery operated device at IIS for rapid and non-destructive assay of ethanol in ethanol-mixed petrol. This development was in anticipation of a possible need for such devices in view of the plan for progressive introduction of ethanol blended petrol throughout the country.

Ethanol, being polar in nature, has dielectric permeability significantly higher than that of petrol. Hence, the dielectric permeability of ethanol-mixed petrol changes as a function of ethanol content. In this device the petrol to be monitored serves as the dielectric medium of a laboratory made capacitor assembly that acts as the timing capacitor of a miniature oscillator circuit. Digital pulse frequency at the output, which can be measured by any hand-held general purpose digital multi-meter, changes sensitively with small change in dielectric strength. An assembly of uniformly spaced rectangular electrodes, immersed in petrol, was used for exploitation of the capacitive effects, and proved to be adequate for monitoring minor shifts in dielectric permeability caused by progressive increase in ethanol level. Thus, for a given device, the shift in frequency from that measured for pure petrol is related to ethanol content.

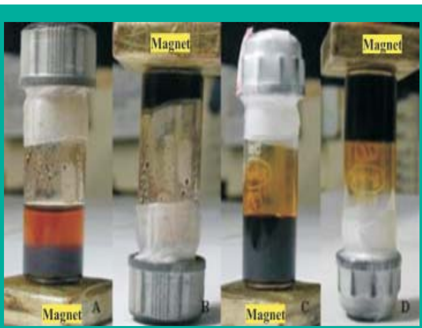
Based on the successful laboratory study, a prototype battery operated unit has been made for field use, a photograph of which is shown in **Fig. 5**. The measured shift in frequency as a function of ethanol content, in the range of 0 – 5 volume percent, is given in **Fig. 6**. Considering the precision of frequency measurement with a general purpose hand-held multi-meter, the measured frequency shifts are quite large, and, therefore, permits sensitive quantitative assay of ethanol in petrol. The range is extendable.

It is to be noted that petrol, being inflammable and highly volatile, was not handled in the laboratory. All measurements related to above data with respect to pure and mixed solutions, including preparation of blended solutions of different compositions for calibration, were completed in about half-an-hour in an open area with this battery operated system, demonstrating its applicability, simplicity and speed for field measurement.

The kit was used to measure the pulse frequencies corresponding to pure petrol samples drawn from seven different petrol bunks around Kalpakkam belonging to Indian Oil, Bharat Petroleum and Hindustan Petroleum companies. The pulse frequencies were practically same and lied within the standard deviation of ±20 Hz (ie ~ 0.06% of the measured pulse frequency). It is seen from the data given in **Fig. 6** that the pulse frequency shifts by more than 200 Hz per volume percent of ethanol. Hence, the ethanol content can be determined easily with good accuracy and precision.

The indigenously developed above inexpensive and non-destructive monitoring devices can be adopted for large scale use in the country for off-line / on-line / field assessment of transformer oil degradation as well as for rapid assay of ethanol in ethanol mixed petrol.

(Reported by B. Saha, Innovative Instrumentation Section, Electronics & Instrumentation Group)



Tailoring of stable ferrofluids for various applications

Ferrofluid is a nanofluid containing magnetic nanoparticles in the size range of 5-10nm. The nano-particles used in ferrofluids are functionalized with organic molecules to prevent agglomeration of particles. The ease of manipulating these fluids by an external field has led to many innovative applications in mechanical, biomedical, electronic and optical systems. Ferrofluids are now used as dynamic mechanical seals, airborne seals for protection of optical devices and sensitive electronic instrumentation in military and surveillance aircraft, heat removal agent, medical applications such as cancer treatment, drug delivery, MRI contrast agents and cell sorting.

The requirement of size, morphology and the magnetic properties of nanoparticles used in the ferrofluid varies with applications. Therefore, the methodologies to control the physical properties of nanoparticles are very important. Among various reproducible synthesis routes for the preparation of nanoparticles, the precipitation technique is one of the most convenient and versatile methods. In precipitation, the nucleated particle size depends on parameters related to reaction conditions, solubility and interfacial energy. Over the last few years, a research programme is being pursued at IGCAR to tailor stable ferrofluids for various applications such as optical sensors, NDT probes and leak free sealant.

Recently, a simple method has developed for tuning the size of the nanoparticles from 2.3 to 6.5 nm by controlling the properties of the solvent media. The nanoparticles with different sizes are prepared by controlling the solubility and reaction rates. The equilibrium critical radius (r*) of particles during nucleation in supersaturated solution is defined as

$$r^* = \frac{2V\sigma}{k_B T \ln(S)} \quad (1)$$

where, V is the molecular volume of the precipitated species, σ is the surface free energy per unit surface area, k_B is the Boltzmann constant, T is the absolute temperature and S is the saturation ratio, which is defined as ratio between solute concentrations at saturation (X) and equilibrium (X_S), i.e. $S = X/X_S$. For a

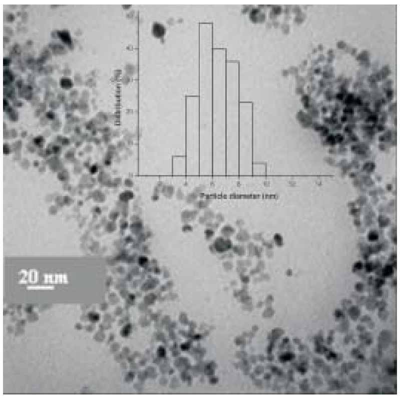


Fig 1. The TEM image of magnetite nanoparticles and the size distribution (inset).

given value of S, all the particles whose radius is below r* will dissolve in the solution whereas others will grow. The concentration X_S of ions forming a saturated solution in equilibrium with the solid is given by

(2)

Where, $\Delta\mu^i$ is the free energy change, a_+ and a_- are radii of ions with charges z_1 and z_2, respectively, e is the elementary charge, ε is the solvent dielectric constant and ε_0 is the permittivity in vacuum. Therefore, the saturation ratio is inversely proportional to the solvent dielectric constant and the equilibrium critical radius is directly proportional to the solvent dielectric constant. By controlling the dielectric constant of solvent with suitable ratio of ethanol to water, it is possible to vary the critical nuclei size and hence the particle size.

By controlling the ratio of ethanol to water, the size of the particles obtained has been varied from 2.3 to 6.5nm where the alkali used for precipitation was NaOH. Table 1 shows the compositions of the solvent, the corresponding particle size and saturation magnetization for the samples S1, S2, S3 and S4. The TEM image of a magnetite sample and the size distribution are shown in Fig 1.

The XRD results show that the samples S1-S4 are magnetite with inverse spinel structure. The inverse spinel structure consists of oxide ions in the cubic close-packed arrangement in which 1/3 of tetrahedral interstices and 2/3 of octahedral interstices coordinate with oxygen. All Fe(II) ions occupy the octahedral interstices, and half of the Fe(III) occupies the tetrahedral interstices and remaining half of the Fe(III) in octahedral interstices. Electron spins of Fe(III) ions in octahedral interstices are aligned anti-parallel to those in tetrahedral interstices. The Fe(II) ions align their spins parallel to Fe(III) ions in adjacent octahedral sites leading to a net magnetization. The measured values of lattice constant for the sample are about 0.838nm. Fig. 2 shows the magnetization curves of samples S1, S2, S3 and S4. All the samples show superparamagnetic behavior with zero remanence and coercivity.

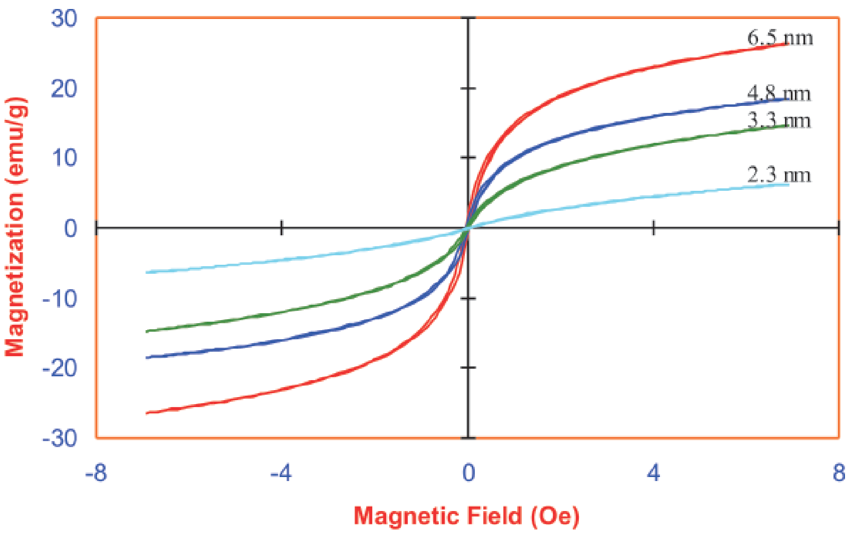


Fig 2: The magnetization curves of samples prepared at different ethanol-water ratio

Table 1

The compositions of the solvent, the precipitated particle size and saturation magnetization..

Sample	*Ethanol: Water ratio*	*Average particle size (nm)*	*Saturation magnetization (emu/g)*
S1	60:40	2.3	6.23
S2	40:60	3.3	14.57
S3	20:80	4.8	18.36
S4	0:100	6.5	26.27

For sealant applications, nanoparticles are functionalized with a monolayer of surfactant molecules. It has been found that, under dynamic coating, a close-packed monolayer of coordinating ligand is formed on the particles, where the surfactant has an ability to control the size and shape of the growing particles. The surfactants provide a primary coating on the magnetite particles, which in turn stabilize the particles against van der Waals and magnetic attraction. The surfactant coated magnetite nanoparticles show a two-step weight loss, where the first weight loss belongs to the weakly bound secondary layer as well as some weaker bound molecules within the primary surfactant layer and the second weight loss belongs to strongly bound primary surfactant layer. The experimental values of weight loss in sample S1 (2.3 nm) and sample S4 (6.5 nm) are 27.6 and 13.6 % respectively. The first loss is observed at ~250°C with small drop of weight and a large drop is observed at ~375°C. Assuming that the surfactant forms a close-packed monolayer on the nanoparticles, the total weight loss due to the loss of surfactant is calculated theoretically. The calculated values of weight loss are found to be 30 and 13.17 % respectively for 2.3 and 6.5 nm sized particles. The experimentally observed amount of surfactant in sample S1 was about 2.03 times more than S4, which was in reasonable agreement with the theoretical calculations (i.e.2.27). The difference between theoretical and experimental values should be attributed to polydispersity of the particles, hindrance effect of surfactant molecules at the interface of small size particles, shape of the particles (in the calculations, particles are assumed to be spherical) and excess free surfactant molecules available in S4. A photograph of magnetite (6.5 nm) based ferrofluids under magnetic field is shown in Fig 3. The samples A & B are unstable under field, due to improper surfactant coating, whereas samples C & D are stable due to a monolayer coating of surfactant on each particle. The nanoparticles suspensions obtained by dynamic coating have shown remarkable stability, in a variety of carrier fluids over very long periods. The in-house developed magnetite based ferrofluids are being used for fundamental studies and sealant applications.

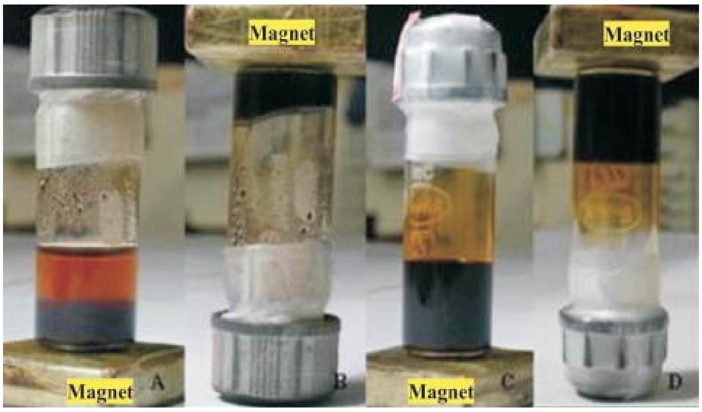


Fig 3: Photograph of magnetite (nanoparticles of average diameter of 6.5 nm) based ferrofluid under magnetic field (i) unstable (A&B) (ii) stable ferrofluid (C&D).

(Reported by John Philip, SMARTS, Non-Destructive Evaluation Division, Metallurgy & Materials Group)

Forum for Young Officers

When non-linearity makes sense: Neural computation in Materials Science

Sumantra Mandal

Mr. Sumantra Mandal obtained his B.E. degree in Metallurgical Engineering from B.E. College, Shibpur in 2002 and M.Tech degree in Materials and Metallurgical Engineering from IIT, Kanpur in 2004 under DAE Graduate Fellowship Scheme (DGFS). He is from DGFS-2002 batch and joined IGCAR as Scientific Officer (SO/C) in September 2004.

Sumantra Mandal and Colleagues, Materials Technology Division, Metallurgy & Materials Group

Artificial neural network (ANN) is a highly simplified model of the structure of a biological network [Fig.1]. The fundamental unit or building block of ANN is the processing element, also called an artificial neuron or simply a neuron. Some neurons interact with the real world to receive input, and some provide the real world with the output. Rest of the neurons remain hidden. Neurons are connected to each other by synapses; associated with each synapse is a weight factor.

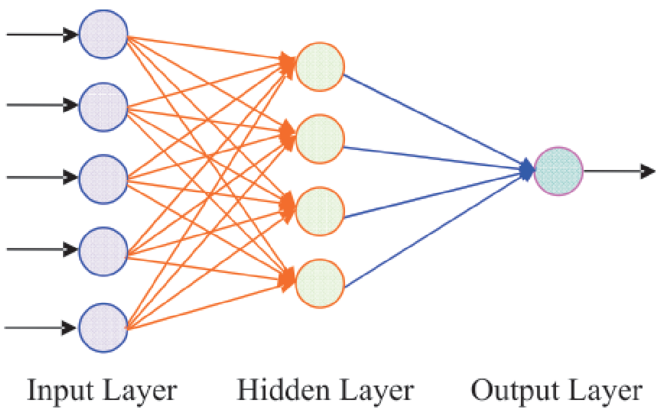


Fig.1: Schematic diagram of feed-forward multilayer neural network

ANN is basically an advance statistical technique that links input data to output using a particular set of nonlinear basis functions. Being a non-linear statistical technique, an ANN can be applied to solve problems that can not be efficiently solved by other conventional statistical model. The basic advantage of employing an ANN approach lies in the fact that they do not require any external manifestation of parametric relationships an ANN learns from examples and recognizes the patterns in a series of input and output values without any prior assumptions about their nature and interrelations. Therefore, ANN can automatically map the complicated relationships between various parameters. These advantages have led to an increased interest in the use of ANN in various fields of materials science.

Constitutive behavior: ANN approach

The constitutive behavior of steel is usually expressed by empirical and semi-empirical relations. However, due to complicated microstructural changes (like work hardening, dynamic recovery and dynamic recrystallization) associated with high temperature deformation processing, it is very difficult to describe the complete hot deformation behavior using a single relationship. Furthermore, development of these models are always time consuming and usually have low accuracy in prediction. In this context, ANN can be considered as an efficient alternative. We have successfully applied ANN to predict constitutive behavior of austenitic stainless steel under hot torsion and compression.

A three layer feed forward network with eight neurons in a single hidden layer and back-propagation learning algorithm has been employed to develop ANN model to predict flow stress under hot compression of alloy D9. Experimental data to train and test the network has been obtained by performing hot compression tests in servohydraulic compression testing machine. The input parameters of the neural network are strain, strain rate and temperature while flow stress is obtained as output. The result of this study shows that coefficient of determination (R^2) for training and test dataset are 0.9937 and 0.9960 respectively. The ANN model for prediction of torsional flow stress for type 304L has been developed employing resilient propagation algorithm. Experimental data to train and test the network has been obtained by performing hot torsion tests in the temperature range 600°C to 1200°C and in the maximum surface strain rate range 0.1 s^{-1} to 100 s^{-1}. The performance of the network for torsional flow stress prediction has been demonstrated in Fig.2.

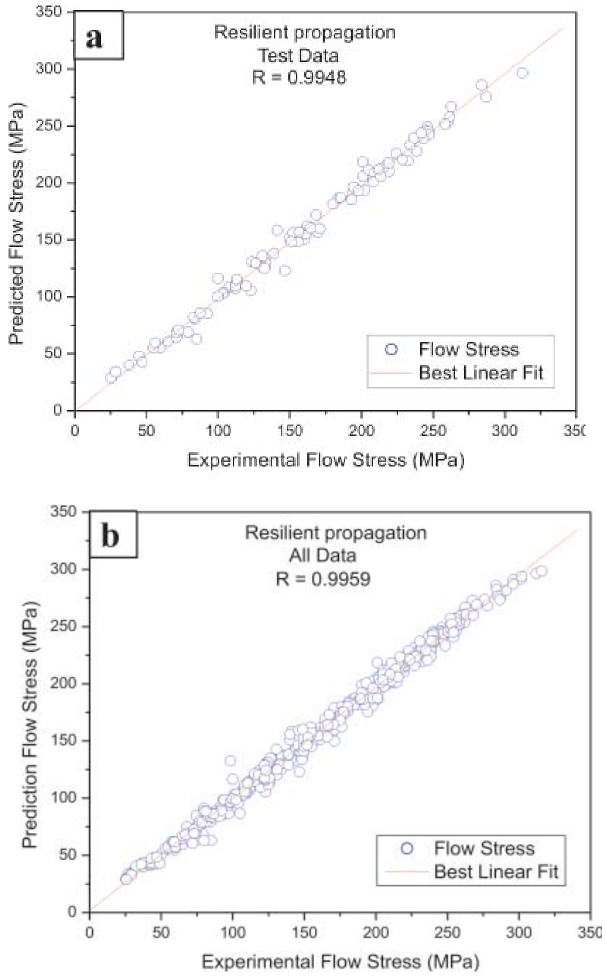


Fig.2: Performance of the network to predict the constitutive behavior of 304L under hot torsion (a) training data set (b) all data set

ANN model to predict microstructural evolution during hot working

A model for the microstructural evolution, including the fraction of dynamic recrystallization (DRX) and grain size, in D9 has been established employing artificial neural network. Microstructural data have been generated through different industrial scale metal forming processes like forge hammer, hydraulic press and rolling in the temperature range 1173K-1473K for various strains. These data have been used to develop the model. The network has been optimized employing resilient propagation and superSAB learning algorithms. The correlation coefficient (R) for test dataset in %DRX prediction is found to be 0.984. The deviation in correlation for grain size data is found to be 5%. However, this magnitude of the error in prediction, in fact, is less than the error that normally arises during grain size measurement. Therefore, it is suggested that the developed model can efficiently predict the microstructural evolution during thermomechanical processing. An instantaneous microstructure, therefore, can be designed in order to optimize the process parameters based on microstructural evolution.

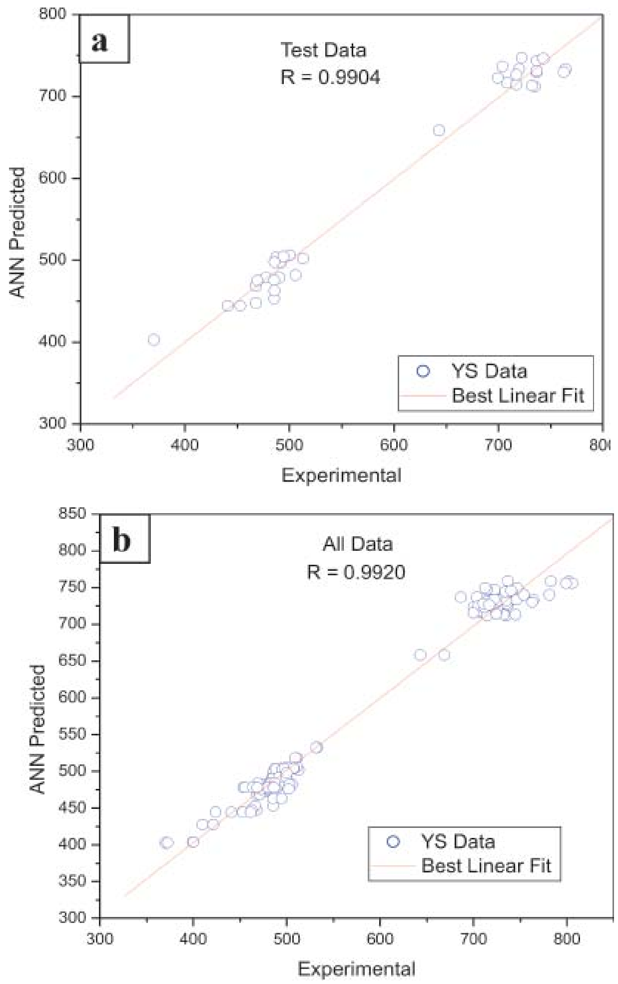


Fig.3: Performance of the ANN model for yield strength (YS) prediction in alloy D9
(a) training data (b) All data

ANN model for tensile property prediction

The mechanical properties of alloy D9 depend on its chemical composition as well as work temperature. It is therefore important to understand the correlation "chemical composition $\Rightarrow$ work temperature $\Rightarrow$ properties", which would eventually help to optimize the alloy composition in order to achieve the desired combinations of properties.

Basically there are two ways to understand such correlations. Firstly, one can construct a physical model that describe the relation between parameters and validate this model with experimental findings. However an explicit physical model that quantitatively describes all the correlations between alloy composition, work temperature and mechanical properties of austenitic stainless steel does not exist. Alternatively, model can be developed applying statistical technique like multilinear regression methods. However, due to synergistic effect of individual alloying elements, the correlation between alloying elements and mechanical properties are highly complex and not simply the sum of the influence of individual element. An artificial neural network model therefore has been developed to simulate the correlation between alloy compositions, test (work) temperature and tensile properties of alloy D9. The input parameters in the model are five alloying elements, C, Ni, Mn, Cr and Mo as well as test temperature. Output parameters are three important tensile parameters namely yield strength (YS), ultimate tensile strength (UTS) and uniform elongation (UE). Different models have been tried and the optimum model has been used for simulation. It has been observed that the developed network is well capable of predicting tensile properties of D9 alloy with sufficient accuracy. The performance of the model for YS prediction is depicted in Fig.3. It can be seen that correlation is quite good and predicted data can efficiently track the experimental findings. The model is recommended for use as a guide line for optimization of alloy composition of alloy D9 in order to achieve desired combination of mechanical properties at different working temperature.

News & Events

IGCAR Awareness Tour and Brain Storming session for Science Teachers of Chennai Colleges

October 2, 2006

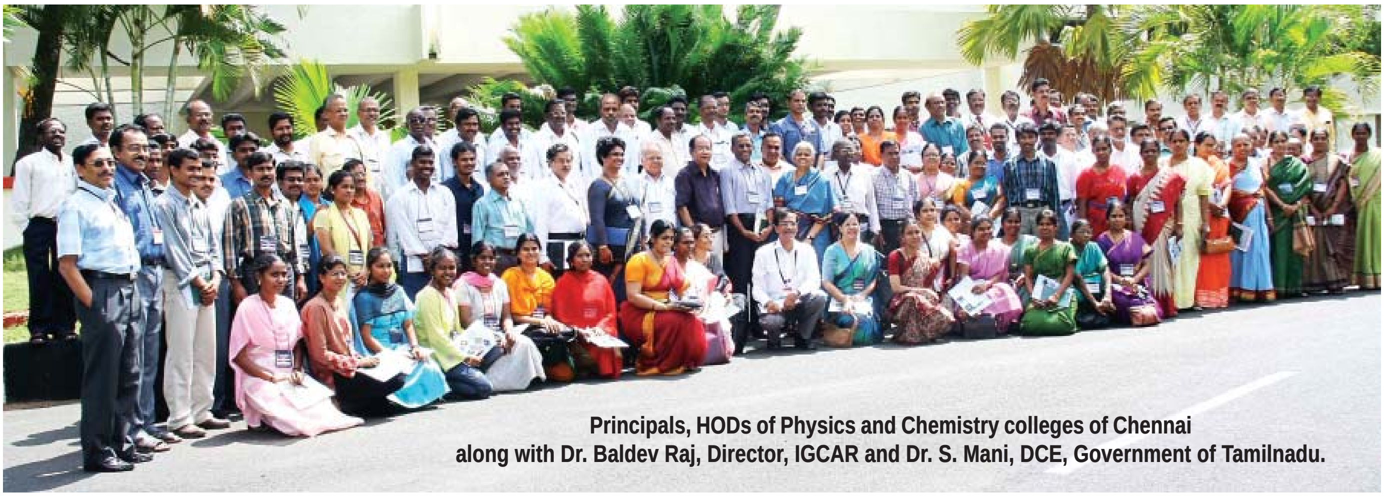
As part of the Centre's sustained initiatives towards improving the quality of science education in universities, and also towards motivating, attracting and retaining the bright young talents in active scientific research, IGCAR organized an awareness tour and a brain storming session with Dr.Baldev Raj, Director, IGCAR for about 140 academia from Madras and Anna Universities, Government and private / Government aided colleges situated in and around Chennai city, in line with the DAE's one of the six key drivers for major programmes viz. mutual strengthening of education and research in nuclear science and technology and allied disciplines. The Chennai team was lead by Dr.S.Mani, Director of Collegiate Education, Government of Tamil Nadu.

Shri P. V. Ramalingam, Director, Reactor Operation & Maintenance Group and also the Chairman of Public Relations Activities Implementation Committee (PRAIC) of IGCAR welcomed the august gathering and presented an overview of DAE. Dr. P. R. Vasudeva Rao, Director, Chemistry, Metallurgy & Materials Groups highlighted the chemistry and physics research programmes of IGCAR. Dr. P. Mohanakrishnan, Head, Reactor Physics Division outlined the reactor physics and safety research activities, Dr. C. S. Sundar, Head, Materials Science Division covered the materials science programme and Dr. K. S. Viswanathan, Head, Analytical Chemistry and Spectroscopy Section spoke on the Centre's chemistry research activities.

A brain storming session was conducted by Dr. Baldev Raj and Dr. S. Mani followed the technical presentations. Dr. Baldev Raj appreciated and complimented the academia for their keen interest and commitment to have participated in the event, despite it being a holiday on account of Gandhi Jayanthi. He shared the concern of the teaching community regarding the declining interest in students to take up science as a career. He critically analyzed the issue and outlined the roadmap to inculcate the scientific temper in the younger generation. He explored the avenues of sharing the excitements of advanced research in physics and chemistry being pursued at IGCAR, and extending the unique and the state-of-the art facilities and infrastructure of IGCAR to the academic world. In his response, Dr. S. Mani appreciated the initiatives and efforts taken by IGCAR, and pledged full support of the TN Directorate of Collegiate Education towards achieving this noble cause. The familiarization tour also identified the domains that require immediate attention, like the need to enhance the employability of science PGs in Indian context.

Visits were conducted in the post-lunch session to the radiochemistry and materials science laboratories and also to the Fast Breeder Test Reactor to enable the academia get first hand knowledge of the experimental facilities and competence of IGCAR. The awareness tour concluded with the panel discussion/ feed-back session conducted by the technical experts consisting of Shri P. V. Ramalingam, Dr. P. R. Vasudeva Rao, Dr. C. S. Sundar and Dr. K. S. Viswanathan. The professors actively participated in the discussion and submitted their written feedback with suggestions for consideration and implementation by IGCAR for reversing the present unhealthy trend. Their suggestions are being compiled and consolidated by the PRAIC. The participants thanked IGCAR for the excellent arrangements in organizing the event and making them familiar with the experimental facilities of IGCAR. Shri J.Daniel Chellappa, Head, Technical Co-ordination & Public Awareness, Chennai and also the Convener of PRAIC proposed vote of thanks and acknowledged the valuable contributions by various agencies involved in this initiative.

(Reported by J.Daniel Chellappa and P.V.Ramalingam, PRAI Committee)



Principals, HODs of Physics and Chemistry colleges of Chennai along with Dr. Baldev Raj, Director, IGCAR and Dr. S. Mani, DCE, Government of Tamilnadu.

Highlights on

Workshop on "Total Quality Management" - November 18, 2006

A one-day workshop on "Total Quality Management (TQM)" was organized by the Madras Library Association, Chennai & MALA-Kalpakkam Chapter on 18-11-2006 at Anupuram Convention Centre. The workshop provided an excellent opportunity to the participants to get to know the evolution and emergence of TQM in their working environment.

Shri M. Somasekharan, President, MALA-KC & Head, SIRD, IGCAR welcomed the gathering and delivered introductory note. Shri M. Rajan, Director, Safety Group inaugurated the workshop and stressed the need to evolve TQM in Libraries. Prof. A. Amudhavalli, President, MALA & Head, Department of Information Science, University of Madras proposed the vote of thanks. Commodore S. Shekar, Managing Director, Sanjeevini Human Resource Institute, Chennai and his team conducted the workshop.

The TQM workshop was designed to give the participants an overview of the all-pervasive nature of Total Quality Management. The workshop was divided into three sessions: Session-1: Introducing TQM, Session-2: TQM Tools and Techniques and Session-3: Putting TQM to work. The workshop was highly interactive and participative. During the final session participants formed five groups and case studies of their choice were presented. The studies were presented and critically evaluated. About 120 delegates from various institutions participated in the workshop. The workshop was highly appreciated by all the participants.

(Reported by M. Somasekharan, SIRD)

Visit of Japanese delegation from Japan Council on Energy and Security (JCES) - November 22-23, 2006

A Japanese delegation led by Prof. Kumao Kaneko from Japan Council on Energy and Security (JCES) visited IGCAR on 22nd and 23rd November, 2006. The members of the delegations were: Prof. Kumao Kaneko, President, JCES, Dr. Osamu Saito, Senior Fellow of JCES, Mr. Makio Tsuji, Senior Fellow of JCES, Mr. Kazuya Ochiai, Fellow of JCES and Dr. Naoyuki Takaki, Fellow of JCES.

The delegation had deliberations with senior scientists of the centre. Dr. Baldev Raj, Distinguished Scientist & Director of IGCAR in his address highlighted the activities of the centre. He also emphasised on R&D approach to FBR with improved economy and safety features. Prof. Kaneko, the leader of the Japanese delegation, talked about the current status of Japanese fast reactor program. The Japanese delegation expressed the hope that the cooperation between India and Japan would be enhanced considerably in the coming years. The delegation visited the Fast Breeder Test Reactor, facilities of the Fast Reactor Technology Group, Safety Group, Structural Mechanics Laboratory, Materials Science Laboratory and PFBR site.

Japanese delegation from Japan Council on Energy and Security, led by Prof. Kumao Kaneko during a discussion meeting with Dr. Baldev Raj, Director, IGCAR and other senior colleagues of the Centre

(Reported by M. Sai Baba, SHRPS)

AWARDS AND HONOURS

Congratulations

- **Dr. Baldev Raj** has been conferred with the honorary Doctor of Science (D.Sc.) by Sathyabama Institute of Science & Technology (Deemed University), Chennai. He has been elected as Honorary Member of Indian Institute of Metals and Honorary Fellow of Indian Welding Society. He has deliverd the following honour lectures, Stanley Ehrlich Distinguished Lecture and Gold Medal, Acoustical Foundation for Education and Charitable Trust, India (2006), International Recognition Award, Indian Society for Non-Destructive Testing (2006)
- **Dr. P. V. Sivaprasad**, Materials Technology Division has been awarded the "Metallurgist of the Year" for the year 2006 by the Ministry of Steel, GOI.
- **Dr A. K. Bhaduri**, Material Technology Division has been elected as the Fellow of Indian National Academy of Engineering from January 2007.
- **Shri P Sukumar,** Non-Destructive Evaluation Division and **Shri N. Vinayagam**, Central Workshop Division, have been awarded the "DAE Meritorious Service Award" for the year 2005.
- **Shri R.Subbaratnam**, QA&NDTS won the prestigious "NDE man of the year Award" for the year 2006.
- STAR Quality Circle of CWD has got the "Distinguished Award" during *20th National Convention of Quality Circle (NCQC-2006)* presentations at IIT, Kanpur, during December 2006.

Dr P.R.Vasudeva Rao, Chairman, Editorial Committee Members: Dr.G.Amarendra, Shri M.Ganapathy, Dr.K.V.G.Kutty, Dr.Mary Mohankumar, Shri G.Padma Kumar, Shri Shekar Kumar, Shri M.Somasekharan, Shri R.Srinivasan, Shri R.V. Subba Rao, Shri K.V.Suresh Kumar. Published by Scientific Information Resources Division, IGCAR, Kalpakkam - 603 102