

भाभा परमाणु अनुसंधान केंद्र का आधिकारिक द्विमासिक प्रकाशन
The official bi-monthly publication of Bhabha Atomic Research Centre



भा.प.अ.के. न्यूज़लेटर BARC Newsletter

जुलाई-अगस्त 2025 July-August 2025 Issue No. 2025:4 ISSN: 0976-2108

● Heavy Water Tech ● Vitrification Annexe Facility ● Trombay Colloquia ● New AKRUTI Kendra

HARNESSING MORE ATOMS
EMPOWERING MORE LIVES...



Mr. Manoj Singh

Mr. Madhav N

Mr. Dinesh J. Vaidya

Ms. Jyoti Panda

Mr. Madhav N



BARC Newsletter
July-August 2025
ISSN: 0976-2108

Newsletter Committee

Dr. A.K. Dureja

Dr. B.K. Sapra

Dr. C.N. Patra

Dr. S. Santra

Dr. S. Mukhopadhyay

Dr. J. Padma Nilaya

Mr. Manoj Singh

Dr. V. Sudarsan

Dr. Tessy Vincent

Dr. S.R. Shimjith

Dr. Sandip Basu

Dr. K.K. Singh

Dr. Kinshuk Dasgupta

Dr. I.A. Khan

Dr. Deepak Sharma

P.P.K. Venkat

Dr. K. Tirumalesh

Dr. Arnab Dasgupta


Dr. S. Banerjee

Dr. V.K. Kotak


Mr. Madhav N



Harnessing More Atoms Empowering More Lives


 Nuclear R&D is advancing at a remarkable pace, blending fundamental research with cutting-edge technology development. Scientific community worldwide, including in DAE institutes such as BARC are deepening their understanding of some of the most intriguing aspects in S&T that are considered to be critical to advancement of nuclear energy and in pursuit of fulfilling 'Net Zero' commitments.

The Department of Atomic Energy, building on its seven decades of remarkable achievements, has outlined a new 'Amritkaal' Vision aimed at scaling newer heights in nuclear power. This Vision aims to reinforce India's global nuclear leadership and improve citizens' quality of life by harnessing the full power of the atom.

 As we move from the notable advancements in nuclear physics and nuclear astronomy within BARC and DAE highlighted in the previous newsletter, this issue showcases some of the interesting multidisciplinary research outcomes from BARC, along with visits from several distinguished guests to our campus.

BARC is intensifying its fundamental research on matter and materials while accelerating technology development to enable faster nuclear reactor deployments through greater collaboration and localization with private sector partners.

As a leading institution, it has the unique opportunity to collaborate with both policymakers and the wider scientific community. Dr. P.K. Mishra, Principal Secretary to the Prime Minister, served as the chief guest at the annual Graduation Function for the flagship OCES Programme 2024 under the auspices of BARC Training School, which marked the induction of 250 successful Scientific Officers.

 At the prestigious Trombay Colloquium, two eminent scientific figures currently serving in the Government of India - Dr. Trilochan Mohapatra and Professor Abhay Karandikar - delivered captivating and deeply insightful talks.

One of BARC's key missions is to showcase its achievements with a broader audience, and this time, senior women scientists were seen leading the outreach efforts in the national capital.

Finally, by harnessing more atoms, we are empowering more lives - ensuring that nuclear science and technology continues to shape a better, more sustainable and equitable future.

Mr. Manoj Singh

Editor, BARC Newsletter &
Head, Scientific Information Resource Division

- **EDITOR'S MESSAGE: Harnessing More Atoms, Empowering More Lives** by Manoj Singh, Editor of BARC Newsletter and Head, SIRD **3**

MULTIDISCIPLINARY NUCLEAR R&D ACTIVITIES

- 1 **Development and Validation of a Code with GUI to Simulate Solute Transport through Liquid Membrane Supported in Hollow Fibre Contactor** **7**
Smita Mishra, K. K. Singh and S. Mukhopadhyay
- 2 **Indigenous Development of Zr-Co based Non Evaporable Getter Pump** **12**
B.K. Das, R. Das, R. Verma and M. Mascarenhas
- 3 **Recent Advances in Indigenous Synthesis of Affordable Organic Ligands for Prostate Cancer Diagnosis** **17**
K. S. Ajish Kumar
- 4 **Mechanical Design and Performance Evaluation of a Laboratory Scale Charcoal Adsorption Column** **24**
A.S.J. Hamilton, M. Srinivas, S. Sukumar and R. Subramaniam

RESEARCH HIGHLIGHTS AND SYNOPSIS

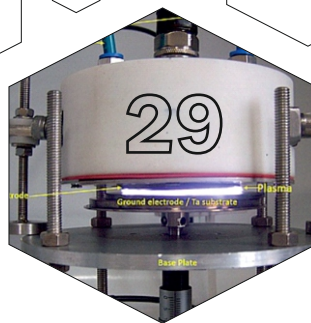
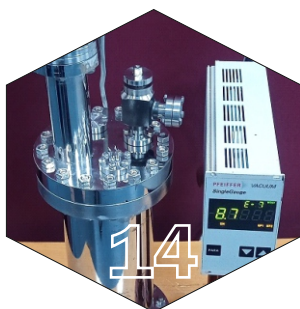
- **Ammonia Activation and Nitride Formation Pathways in Transition Metal Clusters** **28**
Vaibhav Chauhan, Chaithanya Purushottam Bhat, Varun Vinayak Deshpande, Debashis Bandyopadhyay and Soumen Bhattacharyya
- **Cold Plasma Etching Tech for Solid Radioactive Waste Mitigation** **29**
Rajib Kar, R. L. Bhardwaj, J. P. Nilaya and M. L. Mascarenhas

NEWS & EVENTS

- **High hopes from Nuclear Energy as a Source of Clean and Sustainable Power: Dr. P.K. Mishra (Principal Secretary to Prime Minister) said at the Graduation Function of BARC Training School's 68th Batch** **30**
SIRD Newsletter Editorial Team
- **Nuclear Power Expansion Gets Heavy Water Fillip! - Private sector manufactures key components of a nuclear power plant based on BARC technology know-how** **32**
K.T. Shenoy, K. Bhanja, S.K. Bhattacharya and R. Bhattacharyya
- **Strengthening India's Nuclear Waste Management Landscape - Nuclear Recycle Board, BARC hot commissions new Vitrification Annexe Facility at Tarapur** **35**
Subrat Kaushik and K.S. Vasudevan (Nuclear Recycle Board, Mumbai)

TROMBAY COLLOQUIUM:

- **'Transitioning to Ever Green Revolution for enhanced National Food Security' - Excerpts of the talk by Dr. Trilochan Mohapatra, Chairperson of Protection of Plant Varieties & Farmers' Rights Authority (PPVFRA), Govt. of India (AND)** **37**
- **'Securing Advanced & Critical Tech edge for Viksit Bharat' - Excerpts of the talk by Professor Abhay Karandikar, Secretary, Department of Science and Technology, Govt. of India** **38**
SIRD Newsletter Editorial Team

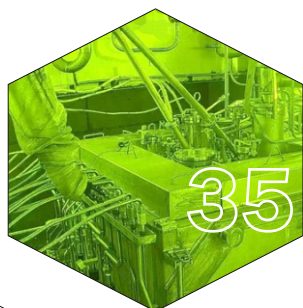


CONNECT

- **Women in 'STEM' empowering Viksit Bharat goal - Senior Women Scientists of BARC drive national outreach on Nuclear Energy Achievements 39**
Dr. Shashwati Sen and SIRD Newsletter Editorial Team

TECHNOLOGY MANAGEMENT

- **Industry Beckons BARC's Nuclear Spin-off Technologies 41**
Technology Transfer & Collaboration Division and SIRD Newsletter Editorial Team



C
O
N
T
E
N
T
S

FORTHCOMING ISSUE

- ▲ Important outcomes across various R&D programmes in BARC.
- ▲ Homi Bhabha Science & Technology Maanpatra (HBSTM).
- ▲ Awards & Honors.
- ▲ News & Events.

This page intentionally left blank

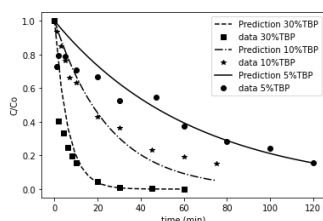
अवअयस्क रेफिनेट से धातु मानों की प्रतिप्राप्ति

1

खोखले फाइबर संस्पर्शित में आलंबित तरल झिल्ली के माध्यम से विलयन परिवहन का अनुकरण करने के लिए जीयूआई के साथ कोड का विकास एवं सत्यापन

एस. मिश्रा*, के. के. सिंह, एस. मुखोपाध्याय

रासायनिक अभियांत्रिकी प्रभाग, भाभा परमाणु अनुसंधान केंद्र (भापअ केंद्र) ट्रांबे, मुंबई-400085, भारत



डेटा वेल्यू के साथ यू (VI) निष्कर्षण के लिए जी. यू. आई. के साथ कोड का सत्यापन

सारांश

खोखले फाइबर संस्पर्शित में प्रयुक्त तरल झिल्ली के उपयोग से विलायक निष्कर्षण प्रक्रमण की तीव्रता के उदाहरणों में से एक है। इस प्रक्रिया द्वारा धातु परिमाणों से क्षीण अम्लीय रेफिनेट का कुशलता से विवेचन किया जा सकता है। यह प्रक्रिया परिमाण प्रतिप्राप्ति और रेफिनेट के कुशल विवेचन, दोनों मामले में लाभदायक है। प्रक्रिया के अभिकल्पन और पैमाने में वृद्धि हेतु खोखले फाइबर संस्पर्शित में सहयोगी/जड़ तरल झिल्ली के माध्यम से द्रव्यमान परिवहन का एक गणितीय मॉडल विकसित किया गया है। वर्तमान शोध-पत्र में, मॉडल समीकरणों को हल करने के लिए ग्राफिकल यूजर इंटरफेस (जीयूआई) के साथ एक कोड विकसित किया गया है और विभिन्न धातु आयनों जैसे कि U(VI), Pu(IV), Cs(I) और Cr(VI) का परीक्षण किया गया है। जीयूआई के साथ कोड धातु आयनों की विभिन्न प्रणालियों, उनके लिगेंड, द्रव-गतिकी स्थितियों एवं संस्पर्शित की विशेषताओं आदि के लिए प्रक्रिया की पूर्वानुमान की सुविधा प्रदान करता है।

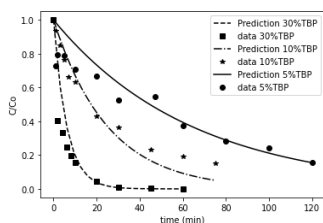
Recovery of Metal Values From Lean Raffinates

1

Development and Validation of a Code with GUI to Simulate Solute Transport through Liquid Membrane Supported in Hollow Fibre Contactor

Smita Mishra*, K. K. Singh, S. Mukhopadhyay

Chemical Engineering Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085, INDIA



Validation of the code with GUI for U(VI) extraction using data

ABSTRACT

Solvent extraction using liquid membrane employed in hollow fibre contactor is one of the examples of process intensification. Acidic raffinates lean in metal values, can be efficiently treated with this process. This process is advantageous in terms of both value recovery and efficient disposal of the raffinate. A mathematical model of the mass transport through liquid membrane supported/immobilized in hollow fibre contactor is developed for design and scale-up of the process. In the present work, a code with graphical user interface (GUI) is developed to solve the model equations and tested for different metal ions viz. U(VI), Pu(IV), Cs(I) and Cr(VI). The code with GUI facilitates prediction of the process for different systems of metal ions, their ligands, hydrodynamic conditions and contactor characteristics etc.

KEYWORDS: Graphical user interface, Hollow fibre contactor, Liquid membrane, Modelling.

*Author for Correspondence: Smita Mishra
E-mail: sdixit@barc.gov.in

Introduction

Hollow fibre liquid membrane process is beneficial for treatment of lean acidic raffinates over conventional process because of its higher interfacial area, non-dispersive contact, modular design and low solvent inventory. Hollow fibre module is a shell and tube type mass transfer contactor, in which a number of thin microporous polymeric fibres are systematically packed in a shell. A fibre is a thin hollow cylinder with wall made of microporous polymer. In the mass transfer process employing hollow fibre contactor, feed flows inside the fibres and strippant flows on the shell side while organic liquid membrane resides in the micropores of the fibre wall. Aqueous-organic interfaces exist at pore mouths. Because of this configuration, simultaneous extraction and stripping occurs at these interfaces. The developed model predicts mass transfer of the metal ion through liquid membrane, for varying operational parameters, using differential mass balance of the solute along a single fibre lumen considering fast interfacial reaction coupled with the solute fluxes through phase interfaces. The details of the model are discussed elsewhere [1]. In this work, a graphical user interface (GUI) of the code to solve the mass transfer model equations is developed. This work is part of ANUSim module development [2] to facilitate prediction of solute transport in solvent extraction contactors.

Methods

The source code of GUI is developed in Python 3.0 interpreter. It predicts concentration profile of metal ion on providing user inputs viz. contactor characteristics (fibre inner and outer diameters, fibre porosity, tortuosity, fibre wall thickness and fibre length), flow rates, distribution coefficients and metal ion diffusivities in aqueous films and organic membrane. Distribution coefficients of metal ions in organic liquid membrane are taken from literature [3, 4]. Individual mass transfer coefficients of feed (aqueous), membrane (organic) and strip (aqueous) are estimated from the reported correlations [5-7] using system parameters. Parameters used for prediction are compiled in Table 1. Experimental data for validation of the model are taken from literature for U(VI) [8-9], Pu(IV) [10], Cs(I) [11] and Cr(VI) [12].

The code with GUI shows the progress of the mass transport with time (t)/ lumen length (z) in terms of concentration profile

of the metal ion. Mass transfer coefficients are estimated and displayed in the GUI. Bench-marking of the code with GUI is done for extraction of different metal ions viz. U(VI), Pu(IV), Cs(I) and Cr(VI).

Results

Fig.1 presents the result of the case study of uranium extraction using the GUI code. Fig.1a shows the prediction made by the model along with the experimental data [8] for different carrier (TBP/ dodecane) concentrations. As carrier concentration increases, rate of uranyl ion transport also increases because of increase in distribution coefficient K_d . Mass transfer coefficient, k_m , decreases with increase in carrier concentration because of increase in viscosity of organic membrane and therefore beyond certain value, increase in carrier concentration will not lead to increase in solute transport in spite of increase in K_d . The predictions are made by using K_d and k_m accordingly as input in the code. Fig.1b presents the plot of model prediction and reported data [9] of uranium transport for a different system having feed acidity of 3N and different strippant with a different hollow fibre contactor having different characteristics. Fig.2 shows the results of plutonium separation for contactor characteristics and system composition given in Table 1 for which model predictions are found in agreement with the reported data [10]. Fig.3 presents the results of the case study of extraction of cesium. Fig.3a shows the prediction of change in dimensionless concentration in feed with time for different feed metal ion concentrations along with the experimental data [11]. As metal ion concentration increases, free carrier concentration decreases at the reaction interface, resulting in decrease in distribution coefficient, K_d at equilibrium. This decrease in K_d leads to decrease in rate of transport as shown in Fig.3a. Model predictions also follow the same trend when varying input value of K_d (shown in Table 1) is used accordingly while executing the code. Figure 3b shows prediction for different feed flow rates along with the experimental data [11]. Prediction (Fig.3b) shows no effect of change of flow rate on metal ion transport (using input of different feed film coefficient, k_f as per different feed flow velocities, v_f). Similar trend of insignificant effect of feed flow rate on extraction has been observed in the experiments [11] and is attributed to the transport rate being membrane diffusion controlled. Fig.4

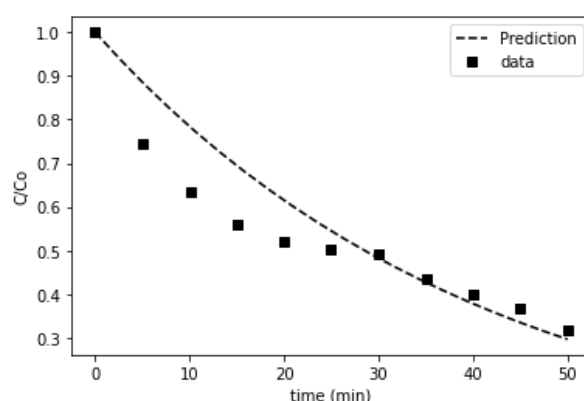
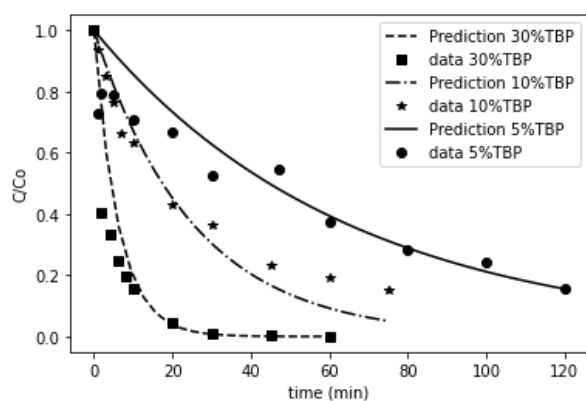


Fig.1: Validation of the code with GUI for U(VI) extraction for (a) data reported in [8], (b) data reported in [9]. The input parameters for the two cases are listed in Table 1.

Table 1: Parameters used for validation case studies

Input Parameters	U(VI)		Pu(IV)	Cs(I)		Cr(VI)
	Case study 1a [8]	Case study 1b [9]	Case study 2 [10]	Case study 3a [11]	Case study 3b [11]	Case study 4 [12]
Fiber outer radius, r_o / inner radius, r_i (cm)	0.015/ 0.012	0.05/ 0.03	0.05/ 0.03	0.015/ 0.012		0.015/ 0.012
Feed flow rate (ml/min)	400	3	3	200	200, 300, 400	840
Feed volume (ml)	500	25	25	500		2000
Feed flow velocity (cm/s)	1.48	0.885	0.885	0.737	0.737, 1.106, 1.4743	3.09
Fiber porosity, ϵ	0.4	0.7	0.7	0.4		0.4
Fiber Pore size (cm), d_p	0.05×10^{-4}	0.2×10^{-4}	0.2×10^{-4}	0.03×10^{-4}		0.03×10^{-4}
Fiber wall thickness, L (cm)	0.003	200×10^{-4}	200×10^{-4}	0.003		0.003
Fiber length, l (cm)	15	10	10	15		15.6
Initial feed metal ion concentration, C_o	0.4 gpl in 1 N HNO ₃	4.6×10^{-3} gpl in 3 N HNO ₃	8×10^{-3} gpl in 3 N HNO ₃	Tracer (1×10^{-7} M), 0.1 gpl in 3 N HNO ₃	Tracer (1×10^{-7} M) in 3 N HNO ₃	0.05-6 gpl at pH 1.5 (0.015N H ₂ SO ₄)
Carrier concentration	30, 10, 5 % v/v TBP/ dodecane	30 % v/v TBP/ dodecane	30 % v/v TBP/ dodecane	1 mM CNC/ 80% NPOE in dodecane		0.213 M secondary amine in Isopar L
Strippant	1 M Na ₂ CO ₃	0.1 M NH ₄ OH.HCl in 0.3 M HNO ₃	0.1 M NH ₄ OH.HCl in 0.3 M HNO ₃	Distilled water		3 M NaOH
Distribution coefficient, K_d	7.66, 1.25, 0.34	26	16	2.13, 1.15	2.13	K_d is function of C_o as, $K_d = -85 \ln(C_o) + 1092$
Feed film coefficient (cm/s), k_f by Leveque correlation $Sh = 1.62 \left(\frac{4r_o^2 v_f}{D_{eff}} \right)^{1/3}$ [5]	1.714×10^{-3}	1.218×10^{-3}	1.218×10^{-3}	3.0858×10^{-3}	3.0858×10^{-3} , 3.53×10^{-3} , 3.882×10^{-3}	2.22×10^{-3}
Membrane mass transfer coefficient (cm/s), k_m by $k_m = \frac{D_{eff}}{L}$ [6,8]	4.733×10^{-5} , 5.6×10^{-5} , 5.8×10^{-5}	1.737×10^{-5}	5.85×10^{-5}	1.467×10^{-5}		3.251×10^{-5}
Strip film coefficient (cm/s), k_s by $\frac{k_s}{v_s} Sc^{0.67} = 3.42 Re^{-0.672}$ [7]	6.33×10^{-3}	1.144×10^{-3}	1.144×10^{-3}	1.1445×10^{-2}		9.3×10^{-3}

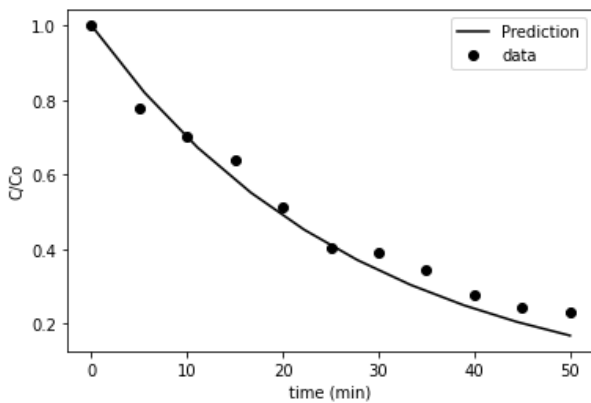


Fig.2: Validation of the code with GUI for Pu(IV) extraction using reported data [10]. The input parameters are listed in Table 1.

shows prediction of chromium flux for different feed chromium concentration with corresponding reported data [12]. As flux is directly proportional to the concentration gradient, increase in feed chromium concentration leads to increase in the flux. Deviation between prediction and data is found ~15% for these case studies. Deviation between model prediction and data is calculated as,

$$\text{Deviation}(\%) = \frac{100}{p} \sum_{m=1}^p \left(\frac{|y_{\text{Expt},m} - y_{\text{Pred},m}|}{y_{\text{Expt},m}} \right)$$

Where, p stands for number of data points and y represents data values. Fig.5 shows the screenshot of the graphical user interface (GUI). The left side of the GUI is for providing user input parameters. The lower middle frame provides the tabs for

Multidisciplinary R&D activities

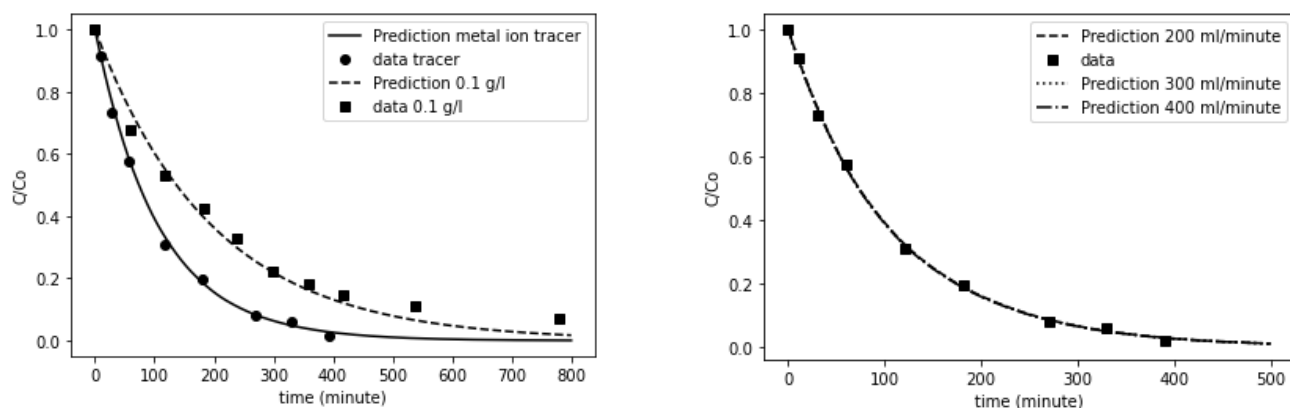


Fig.3: Validation of the code with GUI for Cs(I) extraction for (a) different feed metal ion concentrations (data reported in [11]), (b) different feed flow rates (data reported in [11]). The input parameters are listed in Table 1. Metal ion tracer concentration is 1×10^{-07} M.

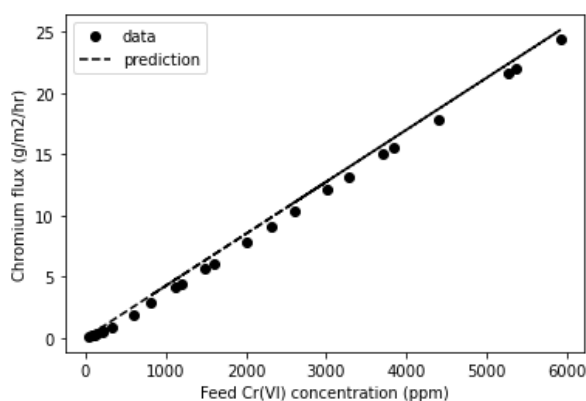


Fig.4: Validation of the code with GUI for Cr(VI) extraction using reported data [12]. The input parameters are listed in Table 1.

calculating mass transfer coefficients and Reynolds numbers after the input parameters have been specified by the user. Pressing the button show graph displays the results in the graphical form on the right side of the GUI. The results obtained from solution of the model equations for the provided user inputs are shown graphically. There is provision to display plots of prediction for both re-circulating (RC) mode and once-through (OT) mode.

In re-circulating (RC) mode, feed is re-circulated through hollow fiber lumen for a definite time, while in once-through (OT) mode, feed is only once passed through the hollow fiber lumen. RC mode displays dimensionless feed concentration in the feed reservoir and % extraction $(=100(1-(C/C_o)))$ versus time, while OT mode displays % extraction versus length of the lumen.

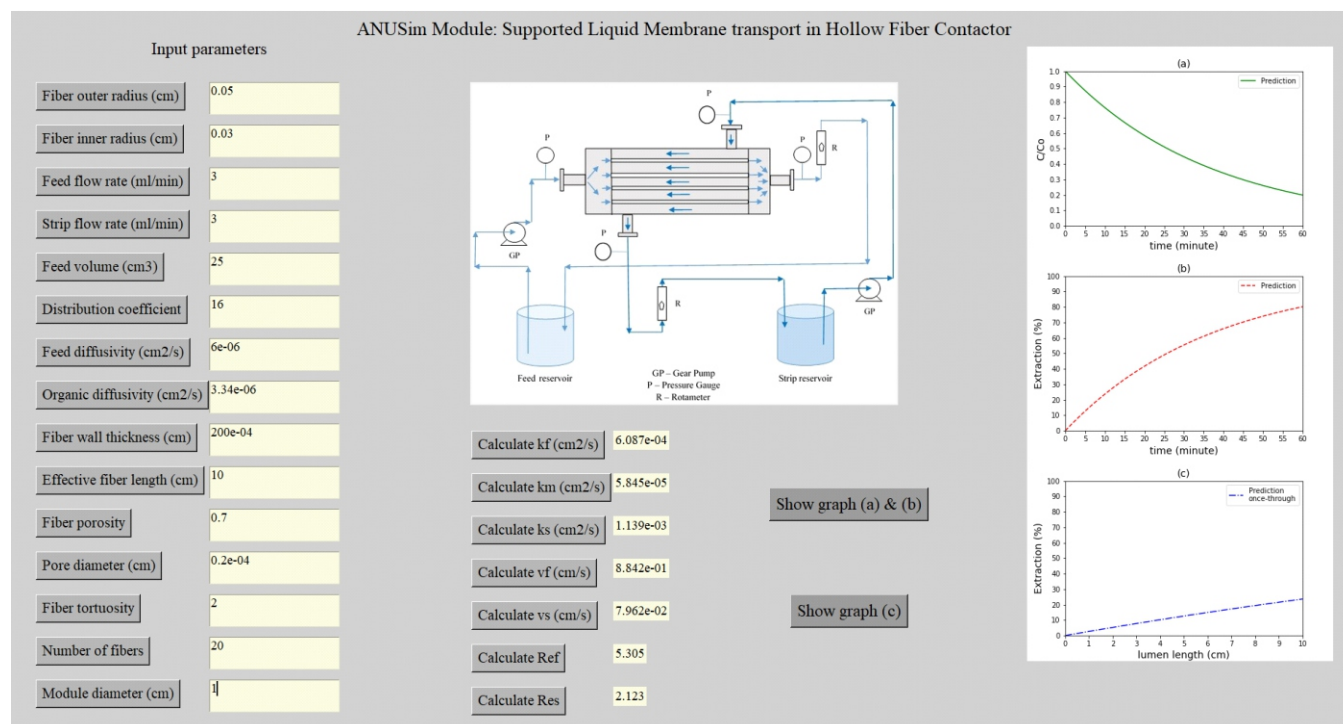


Fig.5: Screenshot of the developed graphical user interface (GUI) of the code for simulating solvent extraction in a hollow fiber module.

Conclusions

Solvent extraction using liquid membrane in hollow fibre membrane contactor is promising for recovery of metal values from lean raffinates. Mathematical model of solvent extraction using liquid membrane in hollow fibre membrane contactor is beneficial for prediction of mass transport process prior to experimental runs. In this work, a code with GUI is developed to simulate the solvent extraction in hollow fibre membrane contactor using supported liquid membrane. The GUI provides the tabs for input parameters to be provided by the user. The model equations are solved in the background and concentration profile of metal ion with respect to time or space are generated. The code with GUI has been validated for extraction of different metal ions (U(VI), Pu(IV), Cs(I), Cr(VI)) with absolute average relative deviation between the predicted and experimental results being ~15%. The code with GUI can be used for parametric analysis and design and scale-up of the process for a given separation task to be achieved using hollow fibre membrane contactor operated in supported liquid membrane mode.

Nomenclature

	Subscript
C - feed concentration	
D - diffusivity	o - initial
k - mass transfer coefficient	aq - aqueous film
K _d - distribution coefficient	org - organic in pores
l - fibre/ lumen length	f - feed
v - flow velocity	m - membrane
Re, Sh, Sc - Reynolds, Sherwood, Schmidt number	s - strip

References

- [1] S. Dixit et al., Desalination and Water Treatment, 79 (2017) 40-48.
- [2] M. Darekar et al., BARC Newsletter, 372 (2020) 21-25.
- [3] O. J. Wick, Plutonium handbook: a guide to the technology, Vol. 1, 1st ed., Gordon and Breach, Science Publishers, New York, 1967.
- [4] S. Dixit et al., Separation Science and Technology, 48 (2013) 2444-2453.
- [5] A. Gabelman, S.-T. Hwang, Journal of Membrane Science, 159 (1999) 61-106.
- [6] E. L. Cussler, Diffusion-Mass Transfer in Fluid Systems, 1st ed., Cambridge University Press, New York, 1988.
- [7] A. Ghazi et al., Chemie Ingenieur Technik, 63 (1991) 381-384.
- [8] S. Dixit et al., Desalination and Water Treatment, 38 (2012) 195-206.
- [9] N. S. Rathore et al., Separation Science and Technology, 39(6) (2004) 1295-1319.
- [10] N. S. Rathore et al., Journal of Membrane Science, 189 (2001) 119-128.
- [11] P. Kandwal et al., Chemical Engineering Journal, 174 (2011) 110-116.
- [12] W.S.W. Ho, T.K. Poddar, Environmental Progress, 20(1) (2001) 44-52.

संलयन प्रौद्योगिकी में संभावित अनुप्रयोग

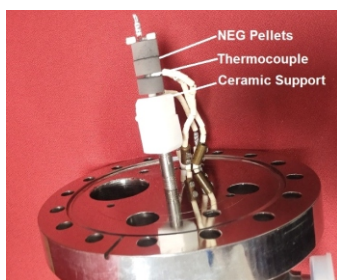
2

Zr-Co आधारित गैर-वाष्पशील गेटर पंप का स्वदेशी विकास

बी.के. दास^{1*}, आर. दास¹, आर. वर्मा^{1,2} और एम. मास्क्रेन्हास¹

¹स्पंद शक्ति एवं विद्युत-चुंबकत्व प्रभाग, भाभा परमाणु अनुसंधान केंद्र, अत्त्युतापुरम, विशाखापट्टणम-531011, भारत

²होमी भाभा राष्ट्रीय संस्थान, अणुशक्ति नगर, मुंबई-400094, भारत



गैर-वाष्पशील जेटरपंप (एनईजी)

सारांश

गैर-वाष्पशील गेटर(एनईजी) का वैज्ञानिक अनुसंधान और उद्योग में अनेक अनुप्रयोग हैं। हमारी प्रयोगशाला में एक लघु गैर-वाष्पीय गेटर पंप विकसित किया गया है। इसमें शुद्ध ज़र्कोनियम और कोबाल्ट पाउडर का उपयोग किया गया। ज़र्कोनियम और कोबाल्ट के मिश्रधातु को मानक सिरेमिक विधि द्वारा पैलेट के रूप में बनाया गया। पैलेटों को एक्स-रे विवर्तन (एक्सआरडी), क्रमवीक्षण इलेक्ट्रॉन सूक्ष्मदर्शी (एसईएम), ताप अपशोषण स्पेक्ट्रमदर्शी (टीडीएस), थर्मोग्रैविमेट्री विश्लेषण (टीजीए) और ब्रुनाउर-एम्मेट-टेलर (बीईटी) द्वारा सेंटरन और अभिलक्षणन किया गया। एक पंप के रूप में इन पैलेटों का परीक्षण एक सीलबंद निर्वात कक्ष में निर्वात उत्पादन हेतु किया गया। ड्यूटेरियम के अवशोषण और अपशोषण में एनईजी पंप की प्रभावशीलता की जांच की गई।

Potential Applications in Fusion Technology

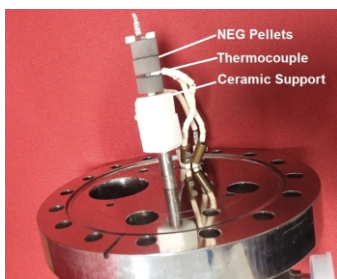
2

Indigenous Development of Zr-Co based Non Evaporable Getter Pump

B.K. Das^{1*}, R. Das¹, R. Verma^{1,2} and M. Mascarenhas¹

¹Pulse Power and Electromagnetic Division, Bhabha Atomic Research Centre, Atchutapuram, Visakhapatnam-531011, India

²Homi Bhabha National Institute, Anushaktinagar, Mumbai, India-400094



Photograph of the NEG pump

ABSTRACT

Non evaporable getter (NEG) has many applications in scientific research and industry. One miniature non evaporable getter pump is developed in our laboratory. Pure zirconium and cobalt powder were used. The alloy of zirconium and cobalt was formed by standard ceramic method in pellet form. The pellets were sintered and characterized by x-ray diffraction (XRD), scanning electron microscope (SEM), thermal desorption spectroscopy (TDS), thermogravimetry analysis (TGA) and Brunauer-Emmett-Teller (BET). The pellets in the form of a pump were tested for generation of vacuum in a sealed off vacuum chamber. The NEG pump was investigated for its effectiveness for absorption and desorption of deuterium. The details about preparation of pellets, characterization and results were discussed in this report.

KEYWORDS: NEG, Getter pump, TGA, BET analysis, Vacuum chamber

*Author for Correspondence: B.K. Das
E-mail: basanta@barc.gov.in

Introduction

Non evaporable getters are used in many scientific applications like, sealed vacuum devices [1], particle accelerators [2], and fusion devices like tokamak [3]. Complex machines like particle accelerators deploy non evaporable getter pumps at inaccessible locations. In recent years non evaporable getter pump has shown as potential equipment for tritium recovery in fusion devices [4]. Non evaporable getter pump is an excellent instrument for production of extreme high vacuum [5]. The active surface of non evaporable getter pumps the residual gases through absorption process. Different gases are absorbed by different processes like chemisorption and physisorption. Reactive gases like oxygen, nitrogen and carbon are absorbed by chemisorption whereas the hydrogen is absorbed by physisorption. The absorption of reactive gases by the NEG is irreversible whereas for hydrogen it is reversible. Though the NEG pumps hydrogen at room temperature, it emits hydrogen at elevated temperature. This property of NEG makes it as a hydrogen source in many applications. Due to their high reactivity, group IV & V elements of the periodic table are used as NEG either in pure form or in the form of alloys. Alloys of titanium, zirconium and vanadium with other elements like iron, aluminum and cobalt are used extensively as non evaporable getter pumps. Alloys are proved to be better NEG than the pure element due to the expansion of the lattice parameters after alloying [6]. Expansion of the lattice parameter becomes favorable for the residual gas atoms to diffuse into the bulk of the NEG.

For the pumping of the residual gases by the NEG, the surface should be active i.e. free from oxide layers. The activation process of the NEG is the important part of its operation. The activation is done by heating NEG to a suitable temperature at which the oxygen at the surface start diffusing in to the bulk. With higher temperature, reactive gases migrate to the bulk whereas hydrogen migrates to the surface and finally emits from it. The NEG pump can be operated for many cycles of pumping and regeneration. The saturation of the NEG pump depends on the capacity to absorb oxygen within itself. During each regeneration, the oxygen from the surface migrates into the bulk thus freeing the surface layer for fresh pumping.

Materials and Methods

For the development of the NEG pump in our laboratory, zirconium and cobalt powder of 99.9% purity were used. General

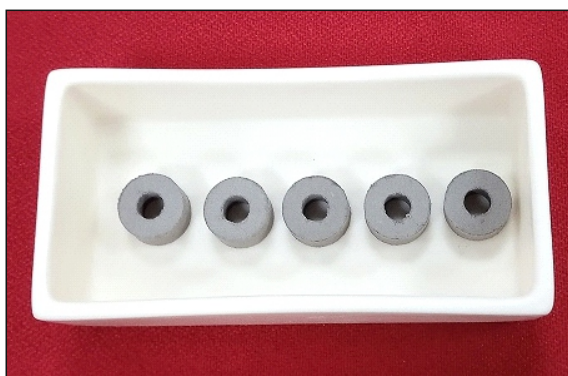


Fig.1: Photograph of Sintered toroidal pellets.

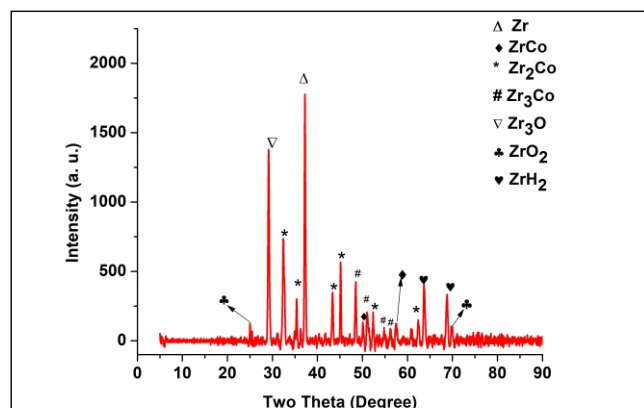


Fig.2: XRD spectrum of the sintered ZrCo Pellet.

ceramic technique was used for alloying. Approximately 5 μm size particles of zirconium and cobalt were taken in wt 70% & wt 30%, mixed well in a vibration mill. The weight percentage of powders was decided after many iterations. The poly vinyl alcohol (PVA) was used as a binder in the mixture. The pellets were formed in pellet die and pressed in a hydraulic press at 3 ton for 5 minutes. The pellets were sintered in a tube furnace at a temperature of 900°C for 1 hour under vacuum of the order of 10^{-2} mbar. The photograph of the sintered pellets is shown in Fig.1.

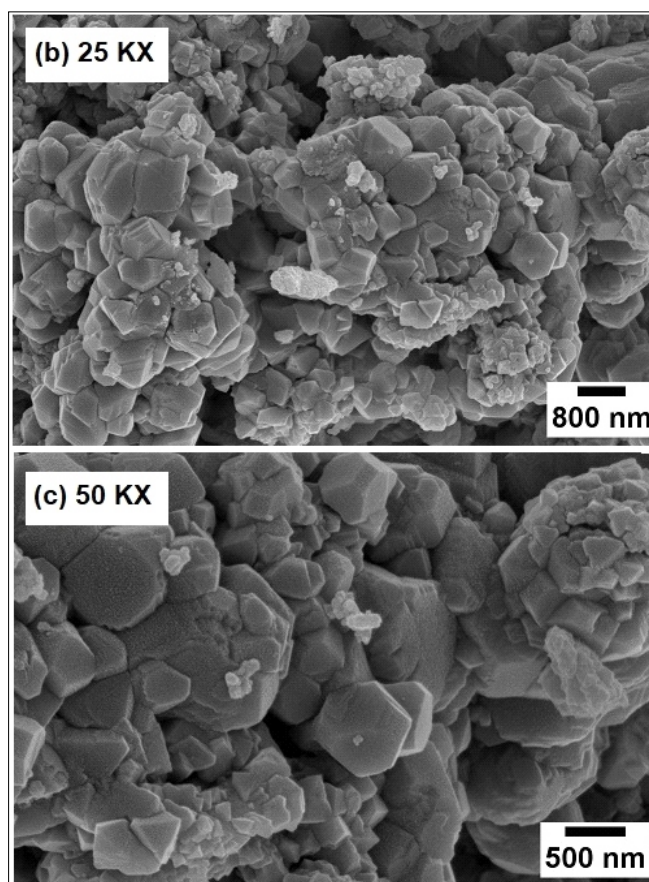


Fig.3: SEM images of sintered ZrCo pellet with magnification of (a) 25 KX and (b) 50 KX.

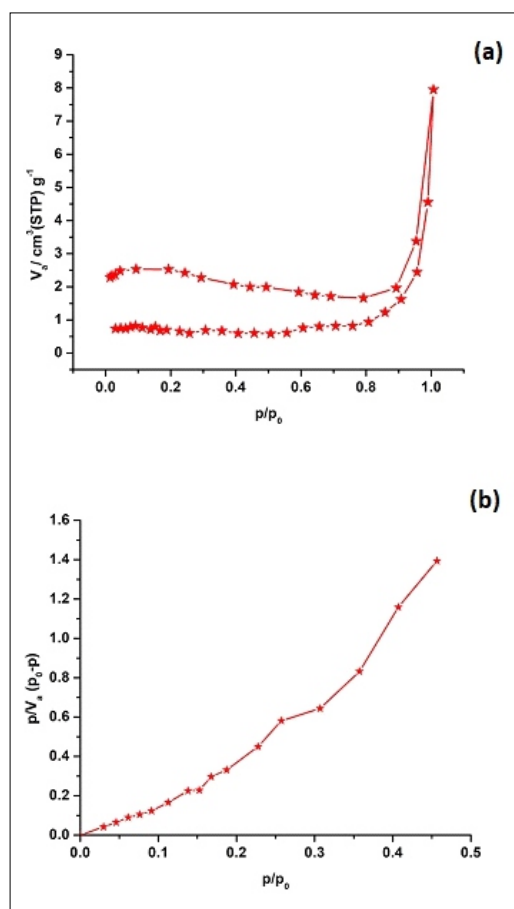


Fig.4: BET analysis (a) adsorption-desorption isotherm, (b) BET plot.

Result and Discussion

Crystallographic study

From the Fig.2, it is observed that the sintered pellet consists of multiple phases of Zr and Co. Phases like ZrCo , Zr_2Co , Zr_3Co and Zr_5O are observed. The lattice parameter of pure Zr is 3.2 \AA whereas that of Zr_2Co is 6.36 \AA , ZrCo_2 is 6.9 \AA and Zr_3Co is 10.84 \AA . The phases having higher lattice parameter like Zr_2Co ,

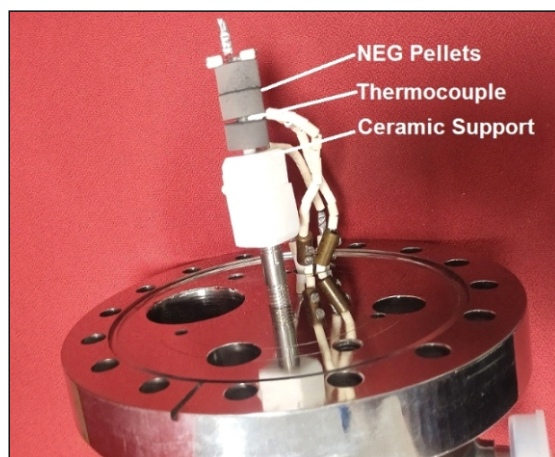


Fig.5: Photograph of the NEG pump.



Fig.6: Photograph of the sealed off vacuum chamber.

Zr_3Co and ZrCo_2 are favorable for gas diffusion into the bulk. Higher lattice parameter facilitates the gas diffusion. These phase formations while alloying of zirconium with cobalt expected to be proved as better non evaporable getter. Apart from different phases of Zr and Co, oxide phases of Zr like Zr_2O and ZrO_2 and hydride phase like ZrH_2 are observed in the XRD spectrum.

Morphology

Fig.3 represents the morphology of the sintered ZrCo pellets observed by scanning electron microscopy. The morphology shows the particles are arranged in manners that of cauliflower like structures with distinguished grain boundaries. Morphology with cauliflower structures due to its higher surface area has great potential for gas adsorption. Average particle size measured by image J software [7] is approximately 437 nm . Closely packed particles are arranged in different planes increasing the surface roughness. There are pores of different geometry. The arrangement of particles in different planes and pores increases the effective surface area of the pellet.

Specific Surface Area

Fig.4 represents plots obtained from Brunauer-Emmett-Teller (BET) analysis. The sample was degassed at 200°C for 1 hour. The analysis was carried out for sample weight of 32.9 mg

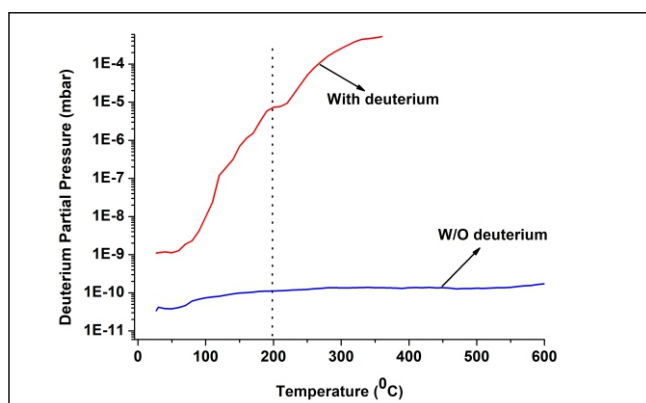


Fig.7: RGA spectrum of deuterium desorption from NEG.

with nitrogen as adsorptive and at adsorption temperature of 77°K. The specific surface area measured from the BET method is found to be 1.68 m² g⁻¹ & total pore volume is 7.07 x 10⁻³ cm³ g⁻¹. The mean pore diameter is 16.747 nm.

Application of NEG Pellets

Sealed Off Vacuum System

Three toroidal pellets with dimensions OD-14 mm, ID-6 mm and height 10 mm were stacked axially in a ceramic insulator with heating elements and mounted on a 16 CF feed through. Total mass of the getters was 14 g and the surface area was 26 cm². The photograph of the NEG pump is shown in the Fig.5. The pump was mounted in a prototype vacuum chamber for testing its effectiveness for generation of vacuum. The prototype vacuum chamber was leak checked with helium leak detector. A gross leak rate of 1.3 x 10⁻⁹ mbar L/sec was observed. The vacuum was created by turbo molecular pump up to a vacuum of the order of 5 x 10⁻⁷ mbar. The NEG was activated at 500°C for 1 hour. The NEG pump was allowed to cool down to room temperature; then the vacuum chamber was isolated from the turbo molecular pump by closing the right angle valve. The sealed off vacuum chamber was pumped only by the NEG pump. The vacuum of the order of 10⁻⁶ to 10⁻⁷ mbar was maintained for more than 2 months and was activated more than 20 cycles till the date of communication of this report. This shows the thermal stability of the NEG pellets. The testing of NEG was done in an unbaked vacuum system. The photograph of the sealed off vacuum chamber is shown in the Fig.6.

Deuterium Replenisher

The getters emit deuterium when heated at elevated temperature [8, 9]. This characteristic of NEG was used to study the present NEG by thermal desorption spectroscopy. The NEG pump was tested for deuterium pumping. The NEG was activated for one hour and allowed to cool down to room temperature at a vacuum of the order of 10⁻⁷ mbar. The NEG was allowed to absorb deuterium gas at a rate of 10 mbar L g⁻¹. After deuterium absorption again vacuum was created by TMP up to 10⁻⁷ mbar of vacuum. At this vacuum, the NEG was heated at a ramp up temperature of 10°C per minute and the partial pressure of the deuterium was measured by residual gas analyzer. The RGA spectrum is shown in the Fig.7. It is observed that with higher

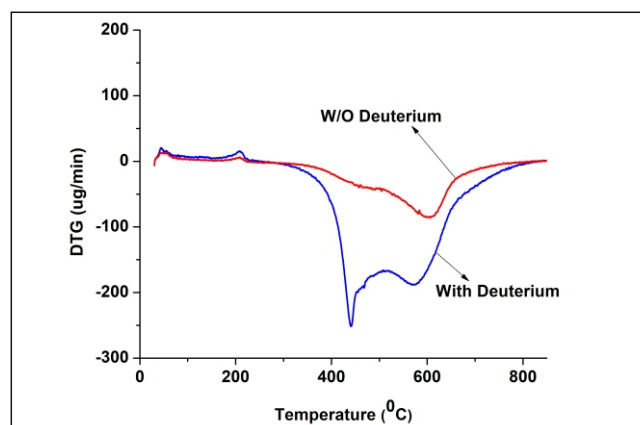


Fig.8: Differential Thermogravimetry plot for ZrCo pellets with and without deuteration.

temperature deuterium starts emitting from the NEG surface.

Tritium Recovery System of Fusion Reactor

NEG based tritium recovery system has been explored for the fusion based reactors [4]. This method is safer than the conventional method. As the temperature of the coolant after the steam generator in fusion reactor is expected to be ~300°C, NEG should absorb tritium at this temperature. To check the applicability of our NEG pellets for tritium recovery systems, the deuterium desorption studies were carried out in differential thermogravimetry. For this analysis deuteration of the NEG pellets was carried out in a dedicated vacuum system [8]. The absorption of deuterium by the NEG pellets was carried out at a rate of 10 mbar L g⁻¹. The differential thermogravimetry plot for the ZrCo pellets with and without deuteration is shown in Fig.8. In case of the deuterated sample, there is abrupt decrease in the mass per unit time after temperature of 314°C. That means deuterium starts to emit from the getter at and after this temperature. This result indicates that the prepared ZrCo could be a potential getter material to be used for tritium recovery system. In our future endeavors detailed study will be carried out to demonstrate the applicability of ZrCo pellets for tritium recovery systems.

Conclusion

For our laboratory applications non evaporable getter is developed based of zirconium and cobalt alloy. Sintered pellets were prepared under vacuum of the order of 10⁻² mbar. XRD spectrum of sintered ZrCo alloy shows formation of multiple phases like Zr₂Co, Zr₃Co characterized by higher lattice parameters which facilitates diffusion of gas into bulk. The morphology taken by SEM shows closely packed grains with pores. Particles arranged in different planes with pores increases the effective surface area. The effective surface area was measured by BET method. The NEG pellets were tested for different applications like sealed off vacuum system, deuterium replenisher and tritium recovery system for fusion reactors. More detail discussions related to the synthesis and characterization of ZrCo pellets is available elsewhere [10].

References

- [1] Sung Hwan Heo, Hyun Jin Kim, Jun Mok Ha, Sung Oh Cho, A Vacuum-Sealed Miniature X-Ray Tube Based on Carbon Nanotube Field Emitters, *Nanoscale Res. Lett.* 7 (2012) 258-262
- [2] C. Benvenuti, A novel route to extreme vacua: the non-evaporable getter thin film coatings, *Vacuum* 53 (1999) 219-225
- [3] H. F. Dylla, A Review of the Wall Problem and Conditioning Techniques for Tokamaks, *J. Nucl. Mater.* 93 & 94 (1980) 61-74
- [4] A. Santucci, L. Farina, S. Tosti and A. Frattolillo, Novel Non-Evaporable Getter Materials and Their Possible Use in Fusion Application for Tritium Recovery, *Molecules*, 25 (2020) 5675
- [5] P. Chiggiato, Production of Extreme High Vacuum with Non Evaporable Getters, *Phys. Scripta.* T71 (1997) 9-13
- [6] A. H. Mogadham, V. Dashtizad, A. Kaflou and H. Yoozbashizadeh, Effect of rare earth elements on sorption characteristic nano structured Zr-Co sintered porous getter, *Vacuum*, 111 (2015) 9-14
- [7] C. A. Schneider, W. S. Rasband and K. W. Eliceiri, NIH Image to ImageJ: 25 years of image analysis, *Nature Methods* 9, 7 (2012) 671-675
- [8] B. K. Das, R. Das, R. Verma, R. Shukla and A. Sharma, Improvement of Deuterium Emission by St 172 NEG Pump in a Sealed off Vacuum Device, *Vacuum*, 181 (2020) 109743
- [9] B. K. Das, R. Das, R. Verma and A. Sharma, Characterization of Deuteriated Titanium Thin Film by Residual Gas Analyzer, *Vacuum*, 196 (2022) 110724
- [10] B. K. Das, R. Das, R. Verma and M. Mascarenhas, Synthesis and characterization of Zr₂Co phase of zirconium-cobalt system, *International Journal of Hydrogen Energy* 111 (2025) 105-112

कैंसर देख-भाल में नवाचार

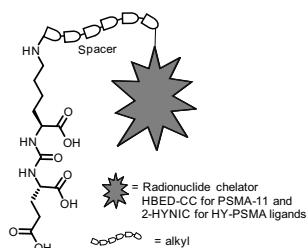
3

प्रोस्टेट कैंसर के निदान हेतु किफ़ायती कार्बनिक लिगेण्ड के स्वदेशी संश्लेषण में हाल में हुई प्रगति

के.एस. अजिश कुमार^{1,2,*}

¹जैव-कार्बनिक प्रभाग, भाभा परमाणु अनुसंधान केंद्र, ट्रॉम्बे, मुंबई-४०००८५, भारत

²होमी भाभा राष्ट्रीय संस्थान, अणुशक्ति नगर, मुंबई-४०००९४, भारत



स्व-गृह संश्लेषित 2-हाइड्राज़िनो निकोटिनिक अम्ल (2-एचवाईएनआईसी) संयुग्मित पीएसएमए लक्षित लिगेण्ड का चित्रण।

सारांश

किफ़ायती नाभिकीय औषधियों को बनाने के लिए स्वदेशीकरण एक अटल कार्यनीति है जो लक्षित रेडियोलिगेण्ड उपचार (आरएलटी) विधि को जरूरतमंदों के लिए सुलभ बना सकती है। दो सामान्य रेडियोलिगेण्ड आधारित नैदानिक विधियों, अर्थात्; एकल फोटॉन उत्सर्जन संगणित टोमोग्राफी (एसपीईसीटी), और पॉज़िट्रॉन उत्सर्जन टोमोग्राफी (पीईटी), में से एसपीईसीटी सबसे व्यापक और सस्ती विधि बनी हुई है। यहाँ, हम उस प्रगति पर चर्चा करेंगे जो हमने एसपीईसीटी और पीईटी आधारित प्रोस्टेट कैंसर निदान के लिए उपयुक्त सिंथेटिक कार्बनिक लिगेण्ड के अनुसंधान एवं विकास में प्राप्त की है। इसके एक भाग के रूप में, स्थापित पीईटी आधारित लिगेण्ड, पीएसएमए-11 के अलावा; एसपीईसीटी आधारित प्रोस्टेट कैंसर नैदानिक लिगेण्ड की मौजूदा आवश्यकता को पूरा करने के लिए, हमने पांच 2-हाइड्राज़िनो निकोटिनिक अम्ल (2-एचवाईएनआईसी) संयुग्मित पीएसएमए लक्षित लिगेण्ड का आंतरिक संश्लेषण किया है।

Innovations in Cancer Care

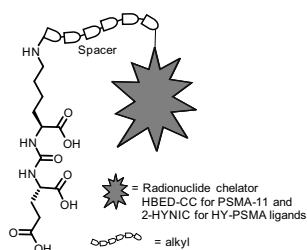
3

Recent Advances in Indigenous Synthesis of Affordable Organic Ligands for Prostate Cancer Diagnosis

K. S. Ajish Kumar^{1,2,*}

¹Bio-Organic Division, Bhabha Atomic Research Centre, Trombay, Mumbai-400085, INDIA

²Homi Bhabha National Institute, Anushakti Nagar, Mumbai-400094, INDIA



Depiction of in-house synthesis of 2-hydrazinonicotinic acid (2-HYNIC) conjugated PSMA targeting ligands.

ABSTRACT

Indigenization is an unswerving strategy to make affordable nuclear medicines that could make the targeted radioligand treatment (RLT) method accessible to the needy. Among the two common radioligand based diagnostic methods, namely; single-photon emission computed tomography (SPECT), and positron emission tomography (PET), SPECT remains the most widespread and affordable method. Here in, we demonstrate the progress that we have attained in the research and development of synthetic organic ligands appropriate for SPECT and PET based prostate cancer diagnosis. As part of it, apart from the established PET based ligand, PSMA-11; to cater the existing requirement for the SPECT based prostate cancer diagnostic ligands, we have materialized in-house synthesis of five 2-hydrazinonicotinic acid (2-HYNIC) conjugated PSMA targeting ligands.

KEYWORDS: Diagnosis, Ligands, Cancer, Prostate, PSMA.

*Author for Correspondence: K.S. Ajish Kumar
E-mail: ajish@barc.gov.in

Introduction

Prostate cancer (PC), a common malignant cancer in men and the second major cause of cancer related deaths is of late showing alarming surge. [1-2] The estimated number of PC cases globally will be ~3 million in a span of next one and half decades [3-5], which would be more than double that was observed in 2020. The surge in the number of cases is also attributed to the advancement in the medical diagnostics, a primary step in the treatment of cancer. Unlike many other human disorders, diagnostic tools are periodically used throughout the course of cancer treatment to estimate the effectiveness of the treatment method adopted. Precise and early stage diagnosis of cancer provides clinicians with the liberty of all available treatment modes. It is perceptible that for such conclusive diagnosis there is still room for the development of diagnostic medicines effective at molecular level. In Indian context, such developments possess great relevance, as India is presently among the cancer hotspots of the world [6,7] due to the significant surge in the number of cancer incidences and associated deaths [8].

Among the existing non-invasive diagnostic techniques; computed tomography (CT), magnetic resonance imaging (MRI) [9], and radio ligand method, the latter is the most sensitive molecular level diagnostic technique, which not only stage the disease but also effectively sketch the treatment progress after cancer therapy. Any effective radio ligand method is based on the manifestation of a biomarker in the targeted cancer cell type. This method is employed in prostate cancer treatment by targeting biomarker, prostate specific membrane antigen (PSMA) or glutamate carboxypeptidase II (GCPII) [10], a type II transmembrane glycoprotein over-expressed on prostate cancer cell surface. To treat prostate cancer through radio ligand method, few effective active pharmaceutical ingredients (APIs), that target PSMA, has been identified and is providing better treatment options for clinicians, globally [11,12]. Unfortunately, most of the APIs used for the radio ligand preparation comes with exorbitant cost, which makes the treatment unaffordable to many patients. PSMA-617 (**1**) and PSMA-11 (**2**), (Fig.1) are few much sought APIs in the therapy and diagnosis, respectively, for prostate cancer management [13-16]. To counter this menace, we initiated the indigenization of APIs along with the development of new APIs for cancer diagnosis and therapy. Over the past 10 years, through our research and development efforts, we successfully undertook the synthesis of some important APIs for radiopharmaceuticals preparations. This includes, three precursors (**3a-c**, Fig.1) for [^{18}F]-FLT (**3**), [17] a positron emission tomography (PET) based brain cancer imaging agent. More recently, few highly important ligands for prostate cancer management, i.e. ligand for endotherapeutic application, PSMA-617 (**1**), PET based diagnostic ligand, PSMA-11 (**2**), and five SPECT based 2-hydrazinonicotinic acid (2-HYNIC) conjugated PSMA ligands, HY-1N-I-PSMA (**4**), HY-2N-I-PSMA (**5**), I-PSMA (**6**), I-1N-PSMA (**7**), HY-Hex-I-PSMA (**8**), through indigenously developed synthetic protocols. When it comes to prostate cancer diagnosis, in addition to the established PET based ligand, PSMA-11, it is always advantageous to have SPECT based PSMA ligand as it would

give another easily accessible tool at the hands of nuclear medicine physicians.

Practically, the main challenge with the PET based medicine, [^{68}Ga]Ga-PSMA-11, is the adequate accessibility of $^{68}\text{Ge}/^{68}\text{Ga}$ generators, [18] which, to an extent can be neutralized with the availability of $^{99}\text{Mo}/^{99\text{m}}\text{Tc}$ generator driven SPECT based PSMA ligands. It is also to be noted that in India, at present, there are only few tens of functional PET scan centres while the number of functional SPECT scan centres are in hundreds. This obviously depicts the need for the development of SPECT based prostate cancer diagnostic agents so that the diagnosis can reach more number of patients at an affordable cost. Among the bifunctional chelators available for radionuclide, $^{99\text{m}}\text{Tc}$, HYNIC is easily synthesizable from cheap and commercially available resources and is also a proven mono-dentate ligand. Therefore, we opted to synthesize analogues of HYNIC conjugated PSMA ligands employing multi-step organic synthesis and investigate their labelling and diagnostic characteristics.

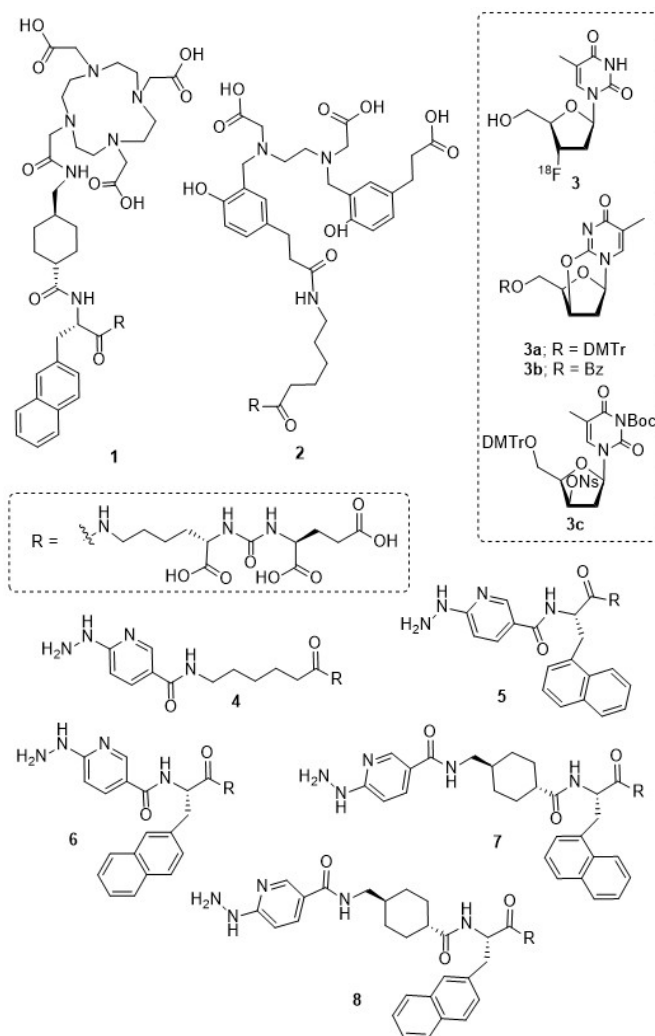


Fig.1: Indigenous organic ligands/precursors: PSMA-617 (**1**), PSMA-11 (**2**), [^{18}F]-FLT (**3**), precursors for [^{18}F]-FLT (**3a-c**), HY-Hex-I-PSMA (**4**), I-1N-PSMA (**5**), I-PSMA (**6**), HY-1N-I-PSMA (**7**), HY-2N-I-PSMA (**8**).

The main objective of synthesizing these ligands through indigenous pathway is to make the radionuclide chelated/conjugated ligand based targeted diagnostic modality, nuclear medicine, affordable to the people of our country. In this account, we demonstrate the synthetic pathways that we have adopted for the synthesis of PET and SPECT based organic ligands, PSMA-11 (**2**), HY-1N-I-PSMA (**4**), HY-2N-I-PSMA (**5**), I-PSMA (**6**), I-1N-PSMA (**7**), HY-Hex-I-PSMA (**8**) (Fig.1), useful for prostate cancer diagnosis, in a cost-effective manner.

Results and Discussion

We initiated the synthesis of PSMA targeting diagnostic ligands program with the synthesis of PSMA-11 (**2**), exercising a homogenous solution phase approach. The rationale behind the same is the leeway of espousing various synthetic strategies, like Fmoc-, Boc-, Cbz- and Alloc-, for efficiently achieving the target molecules. Among the three strategies harnessed for the synthesis of PSMA-11; namely, Fmoc-, Boc-, and Cbz-, we fathomed that the Cbz strategy [13,14] is the most economical in achieving the target. Irrespective of the strategies adopted, when it comes to the synthesis of amino acid based urea containing PSMA targeting ligands, there involves two synthetic segments. The first segment comprised of the construction of the urea template, made from glutamic acid and lysine; which serves as the moiety that binds to the membrane bound protein target, PSMA. To achieve the synthesis of this vital part of the target molecule, one can visualize it through the appropriate selection of differently protected hydrochloride salts (Fig.2) of glutamic acid (**9**), and lysine (**10a**) [13-16]. The selection of the side chain protecting group in lysine, and the protecting group at the amino end in the spacer amino acid would decide the strategy towards the target molecule. The second segment involves synthesis of *N*-protected spacer, which in the case of Cbz-strategy for PSMA-11 is *N*-Cbz protected ω -amino-caproic acid (**11a**), can be

achieved in three steps from commercially available ω -amino-caproic acid [13]. The final coupling constituent in the synthesis of PSMA-11 is the commercially available *t*-butyl protected chelator, HBED-CC.

With the required amino acid precursors (**9/10a/11a**) and HBED-CC in hand, the synthesis of PSMA-11 was initiated. Initially, construction of orthogonally protected urea template (**15a**) was achieved from the appropriately protected hydrochloride salts of glutamic acid (**9**) and lysine (**10a**) as shown in scheme 1, using disuccinimidyl carbonate or triphosgene as the conjugating reagent in the presence of a base. Subsequently, the benzyloxycarbamate (cbz) group in the urea template (**15a**) was removed using 10% Pd/C catalysed flow reactor based heterogenous hydrogenation method to furnish amine (**16**) (Scheme 2), which was coupled to amino acid (**11a**) employing dicyclohexylcarbodiimide (DCC) as coupling agent, to yield the adduct (**17a**). Subjecting (**17a**) for hydrogenation reaction yielded amine (**18**), which on coupling with HBED-CC yielded the fully masked organic compound (**19**). Compound (**19**) on acid hydrolysis furnished the required ligand PSMA-11, in purity >99.5%, post HPLC purification. The structural veracity of the synthesized ligand was compared with commercial PSMA-11 ligand and was found to be equivalent. ^{68}Ga labelling studies conducted at BRIT, Vashi further proved the authenticity of the in-house synthesized PSMA-11. The PET based PSMA tracer, [^{68}Ga]Ga-PSMA-11, made from indigenous PSMA-11, is currently an RPC-approved commercial product of BRIT, Vashi [19].

There is long and successful history for the use of SPECT in diagnostic applications. This single-photon emission based technique is still favoured method among clinicians due to the enormous data available from its practice. Also, SPECT unlike PET is relatively less expensive and hence is popular and easily available in our country too. To date, for prostate cancer diagnosis, no FDA approved SPECT based ligands are globally

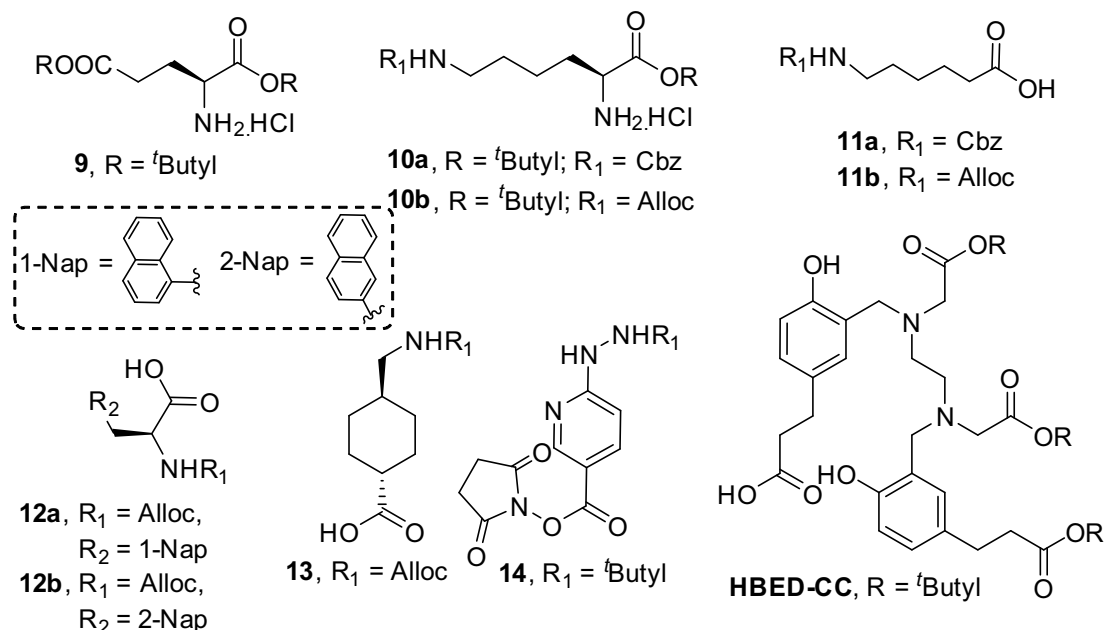
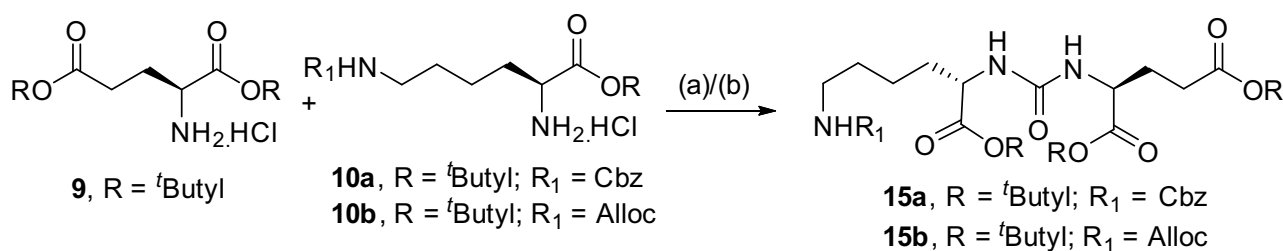
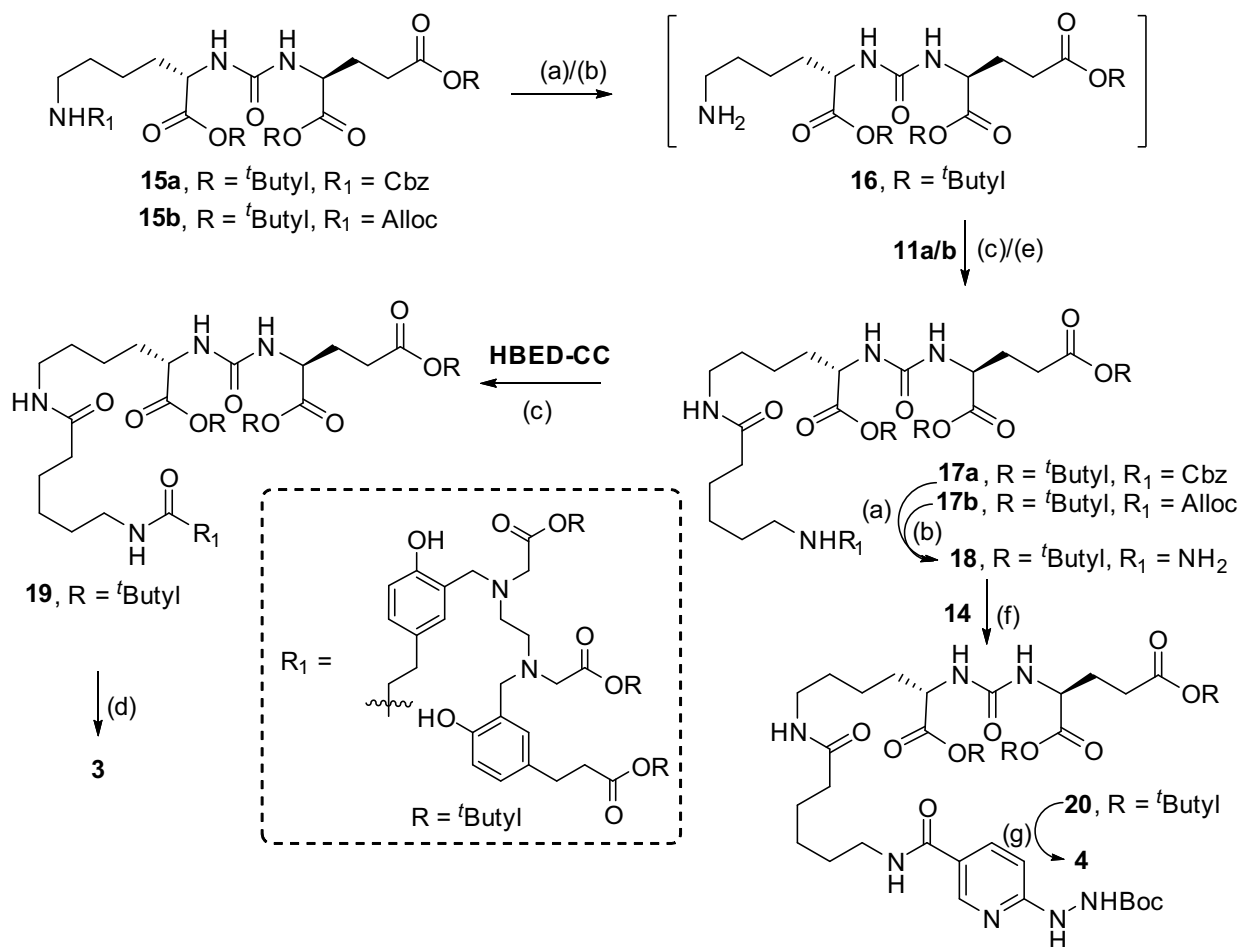


Fig.2: Amino acid constituents/templates for the synthesis of PSMA-11 and HYNIC-PSMA ligands.



Scheme 1: Synthesis of urea templates (**15a/b**): (a) Disuccinimidyl carbonate, DIEA, CH₂Cl₂; (b) CO(OCCl₃)₂, DIEA.



Scheme 2: Synthesis of PSMA-11 (**3**) and HY-Hex-I-PSMA (**4**): (a) 10% Pd/C, H₂ (15 Psi), MeOH; (b) Pd(PPh₃)₄, Phenyl silane, CH₂Cl₂, 25 °C; (c) DCC, DMF; (d) TFA-H₂O-PhSH; (e) HBTU, DIEA, DMF; (f) DIEA, DMF; (g) TFA-H₂O-TIS.

available, even though extensive research efforts are in place, worldwide, to achieve the same [20-25]. ^{99m}Tc being an important γ -emitting SPECT radionuclide, due to its easy availability through ⁹⁹Mo/^{99m}Tc generators [26], favourable physical characteristics (γ = 141 keV; 89% abundance), half-life (T_{1/2} = 6 h), and since various chelator based chemistries are available to complex ^{99m}Tc there is major interest in developing ^{99m}Tc labelled organic ligands for imaging applications. Among various chelators, HYNIC being one of the popular and established bifunctional chelator we pursued the synthesis of HYNIC based PSMA ligands in an attempt to find an appropriate API for SPECT based prostate cancer diagnostic agent. With the above perspective we pursued the synthesis of five 2-HYNIC conjugated PSMA targeting ligands, (**4**), (**5**), (**6**),

(**7**), and (**8**) as shown in Fig.1. Among them ligand (**4**), is the 2-HYNIC variant of PSMA-11, and can be achieved directly from the amine (**18**) by reacting it with the succinimidyl derivative of NBoc-HYNIC (**14**). Alternatively, amine (**18**) can also be accessed through Alloc strategy, as shown in scheme 2, which we have exercised to access all the targeted 2-HYNIC conjugated PSMA ligands. The urea template (**15b**) was achieved by the reaction of glutamic acid derivative (**9**) and lysine hydrochloride derivative (**10b**) (Scheme 1) with triphosgene as the conjugating reagent in the presence of an organic base. Deallylation in (**15b**) was carried out using Pd(PPh₃)₄ to achieve amino compound (**16**) which was coupled with alloc protected ω -caproic acid (**11b**) to furnish (**17b**) (Scheme 2). Deallylation of (**17b**) using aforementioned

palladium catalyst yielded amine (**18**). The reaction of (**18**) with HYNIC reagent (**14**) generated the HYNIC conjugated fully masked adduct (**20**). Acid hydrolysis of triester (**20**) followed by purification using HPLC yielded HY-Hex-I-PSMA (**4**) in desired purity (>99.5%) [27].

For the synthesis of ligands I-1N-PSMA (**5**) and I-PSMA (**6**), the amine (**16**) obtained after the deprotection of alloc group in (**15b**) was subjected to coupling with alloc protected amino acids (**12a/b**) to furnish adducts (**21a/b**) (Scheme 3). In the ensuing step, Pd(PPh₃)₄ catalyzed alloc deprotection in (**21a/b**) followed by conjugation with HYNIC reagent (**14**) under basic condition furnished fully protected compounds (**22a/b**). Acid hydrolysis of (**22a/b**) in the presence of cation scavenger and subsequent HPLC purification afforded (**5**) and (**6**), respectively [27], in the required purity. Ligands (**5**) and (**6**) were characterized using analytical techniques like spectroscopy (¹H/¹³C NMR, IR), HPLC and MS to ascertain their molecular structures [27].

For the synthesis of remaining HYNIC-PSMA analogues, HY-1N-I-PSMA (**7**) and HY-2N-I-PSMA (**8**), the intermediate compounds (**21a/b**) prepared as per scheme 3 was used as the precursors. Following the demasking of alloc group in (**21a/b**), the amines furnished were coupled with alloc protected tranexamic acid (**13**) to yield corresponding compounds (**23a/b**) (Scheme 4). Deprotection of amino group in (**23a/b**), using the reaction condition mentioned before, followed by ligation with HYNIC reagent (**14**) yielded protected ligands (**24a/b**). Global removal of protecting groups in (**24a/b**) under acidic conditions furnished a crude product that on HPLC purification yielded (**7**) and (**8**), respectively, as foamy white solids. The structural integrity and the purity of the isolated product was confirmed by NMR, HPLC and LCMS analysis [27].

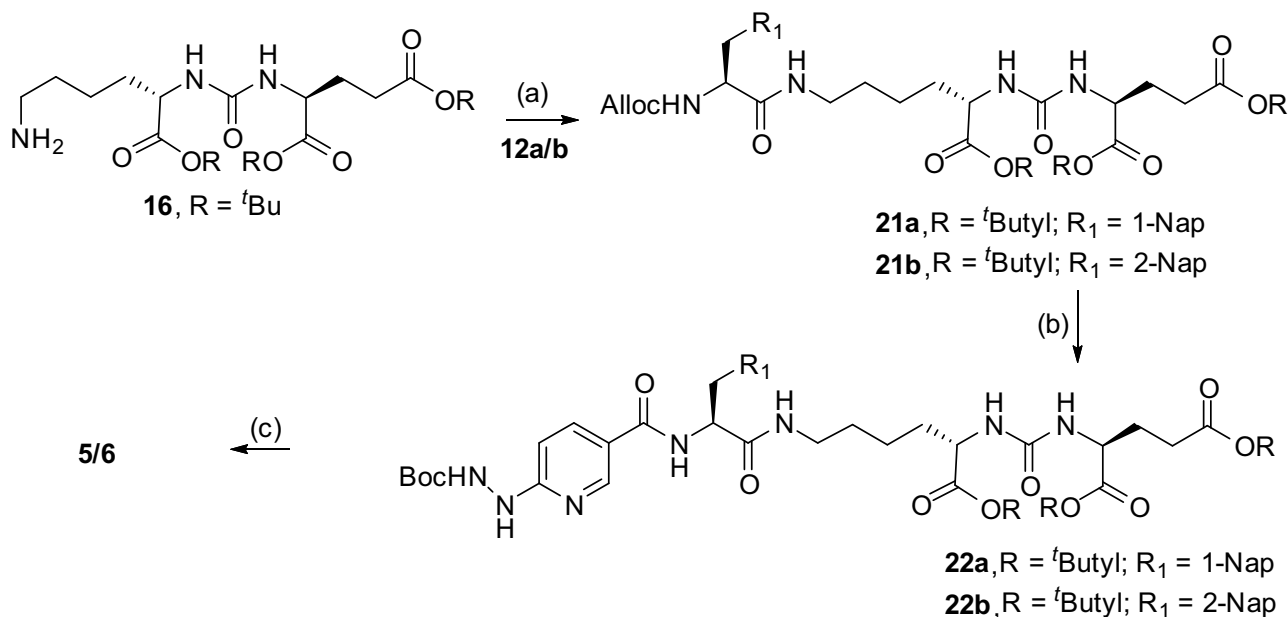
Subsequent to the synthesis of five important 2-HYNIC conjugated PSMA ligands, all the ligands were subjected to

labelling studies using SPECT radionuclide ^{99m}Tc, obtained from ⁹⁹Mo/^{99m}Tc generator, at Radiopharmaceuticals Division (RPhD), BARC. The preliminary labelling studies were encouraging, with two among the five ligands exhibited labelling efficiency greater than 90% sufficient for direct human applications and the other three analogues exhibited >70% labelling efficiency, evoking the requirement of further optimization of labelling conditions [27]. Currently, the synthesized HYNIC-PSMA ligands are in different stages of limited clinical evaluation.

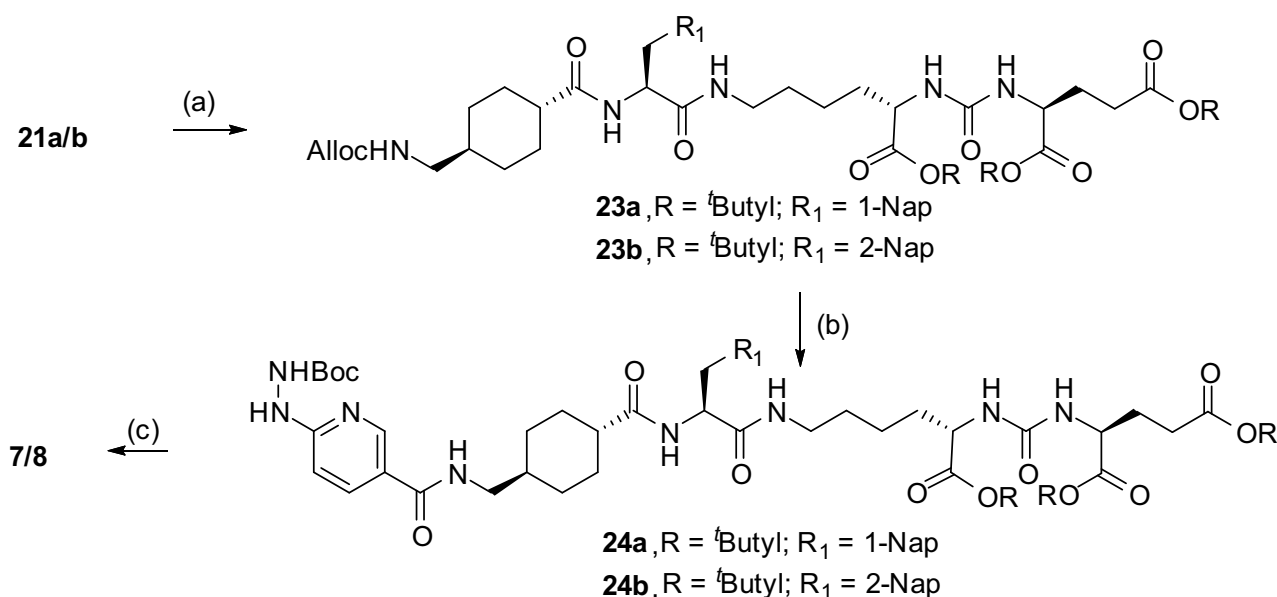
Overall, apart from the pursuit for new ligands for diagnostic applications, through a fruitful collaborative research program with BRIT (Vashi), RMC (Radiation Medicine Centre) and TMH (Tata Memorial Hospital) we were successful in the indigenization of the ligand, PSMA-11, for the preparation of PET based prostate cancer diagnostic agent [⁶⁸Ga]Ga-PSMA-11. These developments are triggered by the success that we savoured with the fully indigenously developed [¹⁷⁷Lu]Lu-PSMA-617, by BOD, BRIT (Vashi), RPhD, RMC, and TMH [28], by virtue of which more than 3000 patients were benefitted through nuclear medicine centres established across India.

Conclusions

Solution phase based Cbz-strategy was found to be an economical method for the synthesis of PET based prostate specific membrane targeting ligand, PSMA-11. Radiolabelling studies of the in-house synthesized PSMA-11 (**2**), carried out at BRIT (Vashi), afforded corresponding labelled products in purity >98% appropriate for direct human applications. Clinical studies conducted at TMH (Parel), using the nuclear medicine, [⁶⁸Ga]Ga-PSMA-11, made from indigenous PSMA-11 ligand, showed results comparable to the commercial equivalents and is currently an RPC approved product. Through the in-house developed synthetic strategy, we are capable of synthesizing the valuable import substitute, PSMA-11, in sufficient



Scheme 3: Synthesis of I-1N-PSMA (**5**) and I-PSMA (**6**): (a) HBTU, DIEA, DMF, 0°C to RT; (b) i) Pd(PPh₃)₄, Phenyl silane, CH₂Cl₂, 25°C; ii) **14**, DMF, DIEA, 25°C; (c) TFA-H₂O-TIS, 25°C.



Scheme 4: Synthesis of HY-1N-I-PSMA (**7**) and HY-2N-I-PSMA (**8**): (a) i) Pd(PPh₃)₄, Phenyl silane, CH₂Cl₂, 25 °C; ii) HBTU, **13**, DMF, 0 °C to RT; (b) i) Pd(PPh₃)₄, Phenyl silane, CH₂Cl₂, 25 °C; ii) **14**, DIEA, DMF, 25 °C; (c) TFA-H₂O-TIS, 25 °C.

quantities with purity >99.5%. In an effort to make SPECT based prostate cancer diagnostic agents we have achieved the synthesis of five 2-HYNIC conjugated-PSMA ligands namely; HY-1N-I-PSMA (**4**), HY-2N-I-PSMA (**5**), I-PSMA (**6**), I-1N-PSMA (**7**), HY-Hex-I-PSMA (**8**), using a solution phase based Alloc-chemistry. Spectroscopic techniques, HPLC, and MS were utilized to establish the structure of the synthesized ligands. Labelling studies using ^{99m}Tc with the synthesized ligands, conducted at RPhD, gave satisfactory results and the fully indigenous [^{99m}Tc]Tc-HYNIC-PSMA tracers are in different phases of clinical evaluation.

Acknowledgments

KSAK is extremely thankful to Prof. B. S Patro, Head, Bio-Organic Division, Prof. P. A. Hassan, Associate Director, Bio-Science Group (BSG) and all the former Group Directors of BSG, particularly, Prof. S. K Nayak, Prof. V. P Venugopalan, Prof. S. K. Ghosh, for their guidance and constant support towards the program. KSAK enthusiastically acknowledge, Prof. Venkatesh Rangarajan (TMH, Parel) for providing clinical data of the studies. KSAK sincerely thank Prof. Sharmila Banerjee (RPhD), Prof. Tapas Das (RPhD), Dr. Usha Pandey (BRIT, Vashi), and Prof. Sandip Basu (RMC, Parel) for their help and support. KSAK is particularly thankful to collaborators, Dr. Madhava B. Mallia (RPhD) and Dr. Anupam Mathur (BRIT, Vashi), for their gusto towards the program. KSAK thankfully acknowledge security personnel of Mod lab for their support.

References

- [1] Wang, et. al, (2022). Prostate Cancer Incidence and Mortality: Global Status and Temporal Trends in 89 Countries From 2000 to 2019. *Front. Public Health*, 10, 811044. doi: 10.3389/fpubh.2022.811044.
- [2] Lu, et.al, (2023). Molecules, Synthesis and Evaluation of ^{99m}Tc-Labeled PSMA-Targeted Tracers Based on the Lys-Urea-

Aad Pharmacophore for Detecting Prostate Cancer with Single Photon Emission Computed Tomography. *Molecules*, 28, 5120. doi: 10.3390/molecules28135120.

- [3] Ferlay, et. al. (2013). Cancer incidence and mortality patterns in Europe: estimates for 40 countries in 2012. *Eur. J. Cancer*. 49,1374-1403. doi.org/10.1016/S0140-6736(24)00651-2.

- [4] James, et. al. (2024). The Lancet Commission on prostate cancer: planning for the surge in cases. *The Lancet Commissions*, 403, 1683-1722. doi:10.1016/j.ejca.2012.12.027.

- [5] Siegel, et. al. (2015) Cancer statistics 2015, *CA Cancer J. Clin.* 65, 5-29. doi:10.3322/caac.21254

- [6] <https://www.apollohospitals.com/apollo-in-the-news/on-world-health-day-apollo-hospitals-has-unveiled-the-4th-edition-of-the-health-of-nation-report>, (accessed Sep 17, 2025).

- [7] Dhillon, et. al. (2018) India State-Level Disease Burden Initiative Cancer Collaborators. The burden of cancers and their variations across the states of India: the Global Burden of Disease Study 1990-2016. *Lancet Oncol.* 19, 1289-1306. doi:10.1016/S1470-2045(18)30447-9

- [8] Sharma, et. al. (2024). Temporal patterns of cancer burden in Asia, 1990–2019: a systematic examination for the Global Burden of Disease 2019 study, *The Lancet Regional Health - Southeast Asia*, 100333. doi:10.1016/j.lansea.2023.100333

- [9] Hövels, et. al. (2008). The diagnostic accuracy of CT and MRI in the staging of pelvic lymph nodes in patients with prostate cancer: a meta-analysis. *Clin. Radiol.* 63, 387-395. doi: 10.1016/j.crad.2007.05.022

- [10] Clarke, et. al. (2010). Markers for detection of prostate cancer. *Cancers*, 2, 1125. doi: 10.3390/cancers2021125

- [11] Maffioli, (2015). Reviews diagnostic And Therapeutic

Management Of Locally Advanced And Advanced Prostate Cancer. *Q. J. Nucl. Med. Mol. Imaging*, 59, 420-438. <https://www.minervamedica.it/en/getpdf/WWRVm0htbVI3NGZTeHR1SE1WQIMyNGdycGJrSGp2cEtQaGIITDBUaTk5S3FoRHlrcWsxdkNzK2Z1RHo5MOpUNg%253D%253D/R39Y2015N04A0420.pdf>

[12] Santoni, et. al. (2014). Targeting prostate-specific membrane antigen for personalized therapies in prostate cancer: morphologic and molecular backgrounds and future promises. *J. Biol. Regul. Homeost. Agents*, 28, 555-563. PMID: 25620167

[13] Theiss, et. al. (1995). Prognostic significance of capsular invasion and capsular penetration in patients with clinically localized prostate cancer undergoing radical prostatectomy. *Prostate*, 27, 13-17. doi: 10.1002/pros.2990270104

[14] Kumar, & Mathur. (2021). Total chemical synthesis of PSMA-11: API for 68Ga-PSMA-11 used for prostate cancer diagnosis. *Eur. J. Med. Chem. Rep.* 3, 100014. <https://doi.org/10.1002/pros.2990270104>

[15] Kumar, & Mathur. (2024). Challenges in the solution phase synthesis of PSMA-11 and PSMA-617: Organic ligands for radiopharmaceutical preparations in prostate cancer medication. *Radiochim. Acta*, 112, 651-662. <https://doi.org/10.1515/ract-2024-0280>

[16] Kumar, & Mathur. (2024). A total chemical synthesis of PSMA-617: A ligand for prostate cancer endotherapeutic applications. *Radiochim. Acta*, 112, 553-563. <https://doi.org/10.1515/ract-2023-0205>

[17] Kumar, & Mathur. (2024). A convenient total synthesis of PSMA-617: A prostate specific membrane antigen (PSMA) ligand for prostate cancer endotherapeutic applications. *Eur. J. Med. Chem. Rep.* 6, 100084. <https://doi.org/10.1016/j.ejmcr.2022.100084>

[18] Kumar, et. al. (2020). BARC Newsletter, November-December-2020.

[19] Hennrich & Eder. (2021). [68Ga]Ga-PSMA-11: The First FDA-Approved 68Ga-Radiopharmaceutical for PET Imaging of Prostate Cancer. *Pharmaceuticals*, 14, 713. doi: 10.3390/ph14080713

[20] Kumar, et. al. (2023). In-house synthesized PSMA-11 as an API for manufacture of 68Ga-PSMA-11 radiopharmaceutical for PET imaging of prostate cancer, May.

[21] Hillier, et.al. (2010). 99mTc-MIP-1340, a small molecule inhibitor of PSMA for molecular imaging of prostate cancer. *J. Nucl. Med.* 51, 481. https://jnm.snmjournals.org/content/51/supplement_2/481

[22] Robu, et. al. (2017) Preclinical Evaluation and First Patient Application of 99mTc-PSMA-I&S for SPECT Imaging and Radioguided Surgery in Prostate Cancer. *J. Nucl. Med.* 58, 235-242. doi: <https://doi.org/10.2967/jnumed.116.178939>

[23] Rathke, et. al. (2018). Intraindividual Comparison of 99mTc-Methylene Diphosphonate and Prostate-Specific Membrane Antigen Ligand 99mTc-MIP-1427 in Patients with Osseous Metastasized Prostate Cancer. *J. Nucl. Med.* 59, 1373-1379. doi: 10.2967/jnumed.117.200220

[24] Papagiannopoulou, (2020). Handbook of Radiopharmaceuticals: Methodology and Applications, M. R. Kilbourn and P. J. H. Scott, Wiley, pp. 375-433.

[25] Urbán, et. al. (2021). Radiation Dosimetry of 99mTc-PSMA I&S: A Single-Center Prospective Study. *J. Nucl. Med.* 62, 1075-1081. doi: 10.2967/jnumed.120.253476

[26] Maurin, et. al. (2022). [99mTc]Tc-PSMA-T4—Novel SPECT Tracer for Metastatic PCa: From Bench to Clinic. *Molecules*, 27, 7216. <https://doi.org/10.3390/molecules27217216>

[27] Hasan, & Prelas. (2020). Molybdenum-99 production pathways and the sorbents for 99Mo/99mTc generator systems using (n, γ) 99Mo: a review. *SN Appl. Sci.* 2, 1782. <https://doi.org/10.1007/s42452-020-03524-1>

[28] Kumar, & Mallia. (2025). Synthesis and radiolabelling studies of hynic conjugated PSMA targeting ligands. *Radiochim. Acta*, 113, 621-636. <https://doi.org/10.1515/ract-2025-0038>.

[29] Kumar, et. al. (2019). ¹⁷⁷Lu-PSMA-617 'Ready to use' Injectable Formulation, September.

प्रभावी उपचार विधि का अभिकल्पन

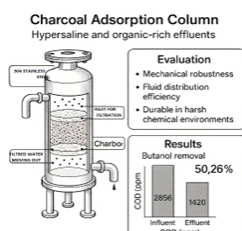
4

प्रयोगशाला स्तर पर चारकोल अवशोषण कॉलम का यांत्रिक अभिकल्पन एवं प्रदर्शन मूल्यांकन

ए.एस.जे. हेमिल्टन^{1*}, एम. श्रीनिवास¹, एस. सुकुमार², जी. वेंकटेशु² और आर. सुब्रमण्यम²

¹बीआईटीएस पिलानी, हैदराबाद, भारत

²भारी पानी संयंत्र, तुतीकोरिन, भारत



सक्रिय कार्बन अवशोषण विधि के लिए चारकोल कॉलम का अभिकल्पन एवं प्रदर्शन।

सारांश

इस अध्ययन में, 304 जंगरोधी इस्पात से निर्मित प्रयोगशाला-स्तर के चारकोल अधिशोषण कॉलम के अभिकल्पन एवं प्रदर्शन मूल्यांकन को प्रस्तुत किया गया है, जो अतिलवणीय एवं कार्बनिक-समृद्ध अपशिष्टों का निपटान करने हेतु अभियंत्रित है। कॉलम का अभिकल्पन यांत्रिक मजबूती एवं द्रव वितरण दक्षता पर बल देता है, जिसमें अनुकूलित ज्यामिति तथा रिक्त स्थान शामिल हैं। विश्लेषणात्मक प्रतिबल-विकृति विश्लेषण तथा परिमित तत्व अनुकरण के माध्यम से यांत्रिक अखंडता को मान्य किया गया। जंग प्रतिरोधी इस्पात कठोर रासायनिक वातावरण में दीर्घकालिक स्थायित्व सुनिश्चित करता है। कॉलम ने जलीय सोडियम क्लोराइड घोल से ब्यूटेनॉल के प्रभावी अपनयन को दर्शाया, जिससे रासायनिक ऑक्सीजन की मांग (सीओडी) 2856 पीपीएम से घटकर 1420 पीपीएम और अपनयन की दक्षता 50.26% हो गई। ये परिणाम औद्योगिक अपशिष्ट जल उपचार के लिए एक स्थायी एवं किफ़ायती समाधान के रूप में चारकोल-आधारित अवशोषण की क्षमता को उजागर करते हैं।

Effluent Treatment Method Design

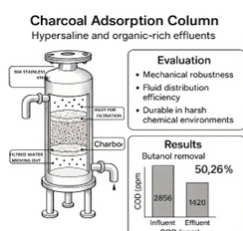
4

Mechanical Design and Performance Evaluation of a Laboratory Scale Charcoal Adsorption Column

A.S.J. Hamilton^{1*}, M. Srinivas¹, S. Sukumar², G. Venkatesu² and R. Subramaniam²

¹BITS Pilani, Hyderabad, INDIA

²Heavy Water Plant, Tuticorin, INDIA



Design and Performance of Charcoal column for Activated Carbon Adsorption Method.

ABSTRACT

This study presents the design and performance evaluation of a laboratory-scale charcoal adsorption column constructed from 304 stainless steel, engineered to withstand hypersaline and organic-rich effluents. The column's design emphasizes mechanical robustness and fluid distribution efficiency, incorporating optimized geometry and void spaces. Mechanical integrity was validated through analytical stress-strain analysis and finite element simulations. The corrosion-resistant stainless steel ensures long-term durability in harsh chemical environments. The column demonstrated effective removal of butanol from an aqueous sodium chloride solution, reducing chemical oxygen demand (COD) from 2856 ppm to 1420 ppm a removal efficiency of 50.26%. These results highlight the potential of charcoal-based adsorption as a sustainable and economical solution for industrial wastewater treatment.

KEYWORDS: COD, Corrosion-resistant, Charcoal, Wastewater

*Author for Correspondence: A.S.J. Hamilton
E-mail: p20220429@hyderabad.bits-pilani.ac.in

Introduction

Activated carbon adsorption columns are vital in environmental remediation and process engineering, particularly for the removal of contaminants from air, water, and industrial effluents [1]. While adsorption efficiency is key to performance, mechanical integrity becomes critical when transitioning from laboratory-scale prototypes to full-scale industrial systems [2,3].

This study focuses on the structural and operational analysis of a charcoal-packed adsorption column fabricated from 304 stainless steel. The column was specifically designed to withstand internal pressures generated by fluid flow and packed bed resistance. Mechanical evaluations including analytical calculations and finite element simulation were conducted to assess hoop and axial stresses, ensuring structural stability under operational loads [4,5].

304 stainless steel was selected for its excellent corrosion resistance, mechanical strength, and suitability for harsh chemical environments, such as those containing organic solvents and hypersaline effluents. The column geometry and packing configuration were optimized to ensure uniform fluid distribution, minimize channeling, and accommodate mechanical stresses.

The column demonstrated effective removal of butanol from an aqueous sodium chloride solution, with the chemical oxygen demand (COD) decreasing from 2856 ppm to 1420 ppm achieving a filtration efficiency of 50.26%. These results underscore the potential of charcoal-based adsorption systems as both mechanically resilient and environmentally sustainable solutions for industrial wastewater treatment.

Materials and Methods

Column configuration and material properties

Material: 304 Stainless Steel – chosen for its excellent corrosion resistance and mechanical strength.

Geometry:

- i. Length: 0.609 m
- ii. Internal Diameter: 2.54 cm
- iii. Total Internal Volume: 0.0002943 m³
- iv. Charcoal Bed Volume: 0.00024531 m³
- v. Top and Bottom Free Spaces: 0.0000490625 m³ and 0.0000294375 m³, respectively.

Load Considerations: The packed charcoal bed density (98.125 g per column) translates into an approximate bulk density, yielding a distributed load over the column's base. The design must account for static loads from the bed as well as dynamic loads from inlet pressure fluctuations.

Flow Distribution and Support Elements

Perforated Plate:

- i. Diameter: 2.54 cm
- ii. Mesh Aperture: 1 mm

These plates are employed at both the inlet and outlet to

ensure uniform distribution across the charcoal bed, helping to mitigate localized overloading and potential mechanical failures.

Mechanical Analysis

The mechanical analysis of the charcoal column includes theoretical stress/strain calculations, finite element analysis (FEA) simulations, and mechanical integrity assessments of both the stainless steel body and the perforated plates.

Analytical stress analysis

For a cylindrical column subject to radial pressure from the packed bed and potential dynamic pressures from fluid flow, the hoop stress (σ_h) and axial stress (σ_a) are of primary concern. These are given by:

$$\text{Hoop Stress } (\sigma_h) = (P.r)/t \text{ and Axial Stress } (\sigma_a) = (P.r)/2t$$

where

P = pressure exerted by the packed bed and fluid flow,

r = internal radius (0.0127 m),

t = wall thickness of the column (assumed based on design; e.g., 1–2 mm).

For instance, if an internal pressure of 50 kPa is assumed during peak operation, the calculated stresses (0.635 MPa and 0.3175 MPa) ensure that the design remains within the allowable stress limits for 304 stainless steel, typically around 205–240 MPa in bending and tensile modes.

The Fig.1 demonstrates the cylindrical geometry, indicating the internal radius, wall thickness, and load-induced stress vectors. The figure highlights the hoop (circumferential) and axial stresses with annotated equations.

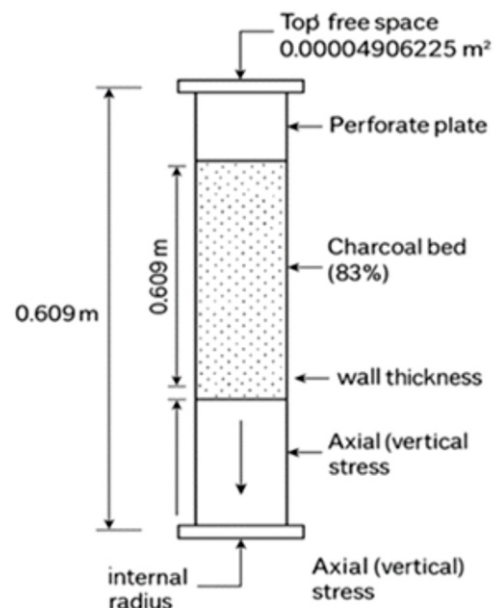


Fig.1: Conceptualized Charcoal column geometry.

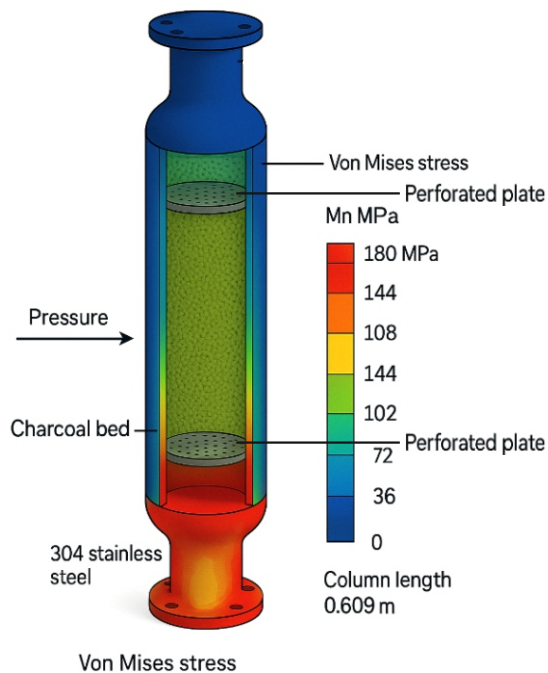


Fig.2: FEA Analysis of Charcoal column using Ansys.

Finite element analysis (FEA) simulation

Complementing the analytical calculations, an FEA simulation was conducted to visualize the stress distribution over the column wall under operational load conditions. The simulation assumed:

- Boundary Conditions: Fixed constraints at the base; distributed pressure corresponding to the packed bed and transient flow conditions.
- Stress Concentration Areas: Around the perforated plates and the free spaces.

A color-coded stress in Fig.2 of the column wall and support plates is provided. The diagram shows peak stress regions, with particular attention to the transitional zones near the perforated plates. This simulation validates that the maximum stress levels remain below the yield strength of 304 stainless steel, confirming the structural reliability under both static and dynamic loads.

Strain analysis and deformation

Small deformations are expected due to the stiffness of stainless steel. Strain (ϵ) analysis based on Hooke's Law ($\epsilon = \sigma/E$) indicates that the maximum computed strains are in the order of 10^{-4} to 10^{-3} , where E (Young's modulus) for 304 stainless steel is approximately 193 Gpa. Both analytical and simulated strain values confirm negligible deformation, ensuring the integrity of the adsorption process.

The strain distribution along the column height in Fig.3 localized strain values near structural discontinuities, such as the edges of the perforated plates and the interfaces of the free spaces, reinforcing the robustness of the design.

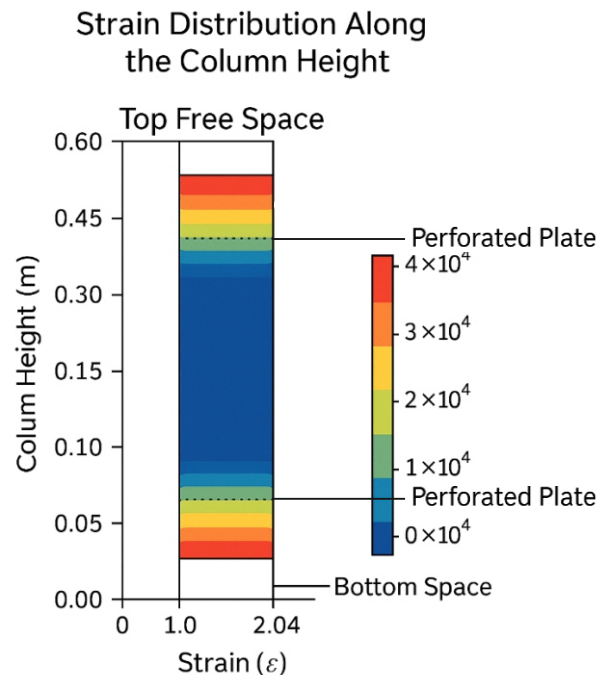


Fig.3: Strain Distribution in charcoal column using Ansys.

Filtration Efficiency of Charcoal filter bed

The charcoal adsorption column demonstrated effective removal of butanol traces from an aqueous sodium chloride solution, resulting in a substantial reduction in chemical oxygen demand (COD). The initial COD of the solution was 2856 ppm, primarily attributed to the presence of organic butanol compounds. Following treatment through the charcoal-packed column, the COD was reduced to 1420 ppm, indicating significant adsorption of organic contaminants by the charcoal media. This corresponds to a filtration efficiency of approximately 50.26%, highlighting the potential of charcoal-based adsorption as a cost-effective and environmentally sustainable method for treating organic-laden industrial effluents.

$$\text{Filtration Efficiency (\%)} = \frac{(\text{Initial COD} - \text{Final COD})}{\text{Initial COD}} \times 100$$

$$= \frac{(2856 - 1420)}{2856} = 50.26 \%$$

Discussion

The combined analytical and numerical results validate the mechanical viability of the charcoal adsorption column design. The low induced stress and strain levels confirm that both the column wall and the perforated support plates can safely withstand operational pressures without risk of permanent deformation. Uniform stress distribution across the structure minimizes the potential for mechanical failure or leakage an essential factor for scale-up in industrial applications [6]. The incorporation of free spaces enhances flow uniformity and adsorption contact without compromising structural integrity, aligning with prior findings on packed-bed reactor optimization [7,8].

The system also demonstrated effective contaminant removal. The column achieved a filtration efficiency of approximately 50.26%, reducing the COD of a butanol-contaminated saline solution from 2856 ppm to 1420 ppm. This performance is consistent with other studies reporting the efficacy of activated carbon in removing organic solvents from aqueous solutions. The favorable flow dynamics supported by the optimized geometry likely contributed to improved mass transfer and adsorption efficiency, a factor well-documented in porous media flow studies [9].

Finite element analysis (FEA) corroborated theoretical stress predictions, reinforcing confidence in the column's mechanical design and long-term reliability [10]. Collectively, the analysis highlights the potential of this system as a scalable, dual-performance solution for industrial wastewater treatment offering both structural durability and environmentally sound treatment of hypersaline, organic-laden effluents.

Conclusions

The designed charcoal adsorption column successfully integrates mechanical integrity with effective contaminant removal performance. The comprehensive mechanical analysis encompassing stress and strain evaluations through both analytical methods and finite element analysis confirms that the column, fabricated from 304 stainless steel, is structurally sound and capable of withstanding the operational pressures encountered during treatment of hypersaline, organic-laden effluents.

In addition to mechanical reliability, the column demonstrated notable treatment efficiency, achieving a 50.26% reduction in chemical oxygen demand (COD) when processing a butanol-contaminated saline solution. This level of filtration efficiency highlights the potential of activated charcoal as a practical medium for removing organic pollutants under challenging chemical conditions.

Further experimental validation, including pressure drop measurements and dynamic load testing, is recommended to

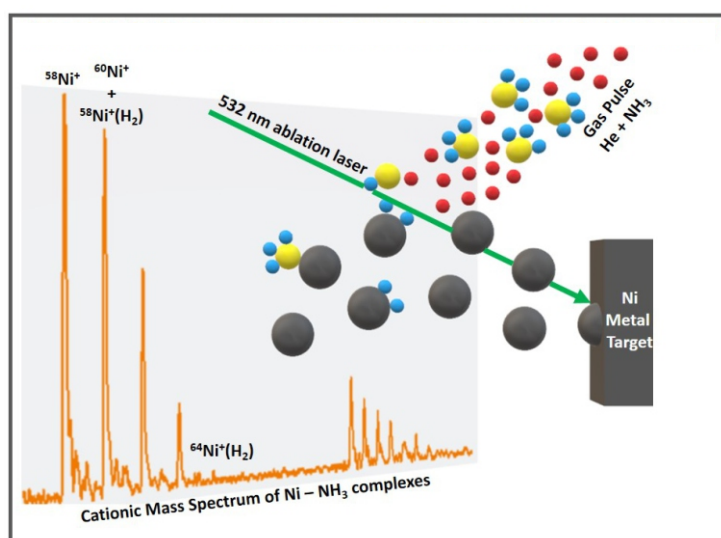
fully characterize performance under real-world operational scenarios. The approach outlined in this study provides a robust foundation for scaling the system for industrial wastewater treatment applications, combining structural durability with environmentally sustainable treatment capabilities.

References

- [1] Ruthven, D. M. Principles of Adsorption and Adsorption Processes. Wiley, 1984.
- [2] Bansal, R. C., & Goyal, M. Activated Carbon Adsorption. CRC Press, 2005.
- [3] Perry, R. H., & Green, D. W. Perry's Chemical Engineers' Handbook. McGraw-Hill, 2008.
- [4] ASTM Standard for Pressure Vessels – Guidelines on pressure-induced stress evaluations.
- [5] Timoshenko, S. P., & Goodier, J. N. Theory of Elasticity. McGraw-Hill, 1970.
- [6] Smith et al., 2018, Design and Analysis of Pressure Vessel Subjected to Pressure Loading. International Journal of Engineering, 2018.
- [7] Zhang, Y., Li, Z., Chu, G., Shao, L., Luo, Y., & Chen, J. Liquid–solid mass transfer in a rotating packed bed reactor with structured foam packing. Chinese Journal of Chemical Engineering, 2020.
- [8] S.M. Chelate, V.S. Kamble. Adsorption and Kinetic study of priority organic pollutant phenol from aqueous waste using Activated carbon. Journal of Advanced Zoology 2020.
- [9] D.M. Nevskaya, A. Jerez, et.al., Porosity and Adsorption Properties of an Activated Charcoal. Colloids and Surfaces: A Physicochemical and Engineering Aspects 2001.
- [10] Yoshiaki Goto, Kosuke Mizuno, et.al., Nonlinear Finite Element Analysis for Cyclic Behavior of thin-walled stiffened rectangular steel columns with infilled concrete, Journal of Structural Engineering, 2012.

Designing of Efficient Catalysts

Ammonia Activation and Nitride Formation Pathways in Transition Metal Clusters



Ammonia activation by transition metal clusters, linking chemistry to hydrogen energy.

Vaibhav Chauhan¹, Chaithanya Purushottam Bhat², Varun Vinayak Deshpande^{1,3}, Debashis Bandyopadhyay², and Soumen Bhattacharyya^{1,3,*}

¹Atomic & Molecular Physics Division, Bhabha Atomic Research Centre, Trombay, Mumbai – 400085

²Physics Department, Birla Institute of Technology & Science, Pilani – 333031

³Homi Bhabha National Institute, Anushakti Nagar, Mumbai – 400094

*E-mail for Correspondence: sbhatt@barc.gov.in

This study provides new mechanistic insights into the pathways of ammonia activation and transition metal nitride formation at the nanoscale. The results not only enhance fundamental understanding of cluster reactivity but also offer guiding principles for the rational design of efficient catalysts for hydrogen production and nitrogen cycle processes.

The figure displayed at the top depicts the reaction products of a few transition metal clusters (V, Ti, Ni, Co, & Fe) with NH_3 gas in a laser vaporization source.

Ammonia (NH_3) is a key hydrogen carrier and a vital feedstock for fertilizers, yet its decomposition and activation pathways remain challenging in catalysis. Transition metal (TM) nitrides have recently emerged as promising alternatives to noble-metal catalysts, offering high activity, stability, and lower cost. To gain atomistic insights into ammonia activation, a combined experimental and theoretical study was carried out at the Atomic and Molecular Physics Division, BARC.

In this work, laser-vaporized clusters of Ti, V, Fe, Co, and Ni were generated and their reactions with ammonia were investigated using reflectron time-of-flight mass spectrometry (ReTOFMS). Complementary density functional theory (DFT) calculations were employed to unravel the underlying reaction pathways.

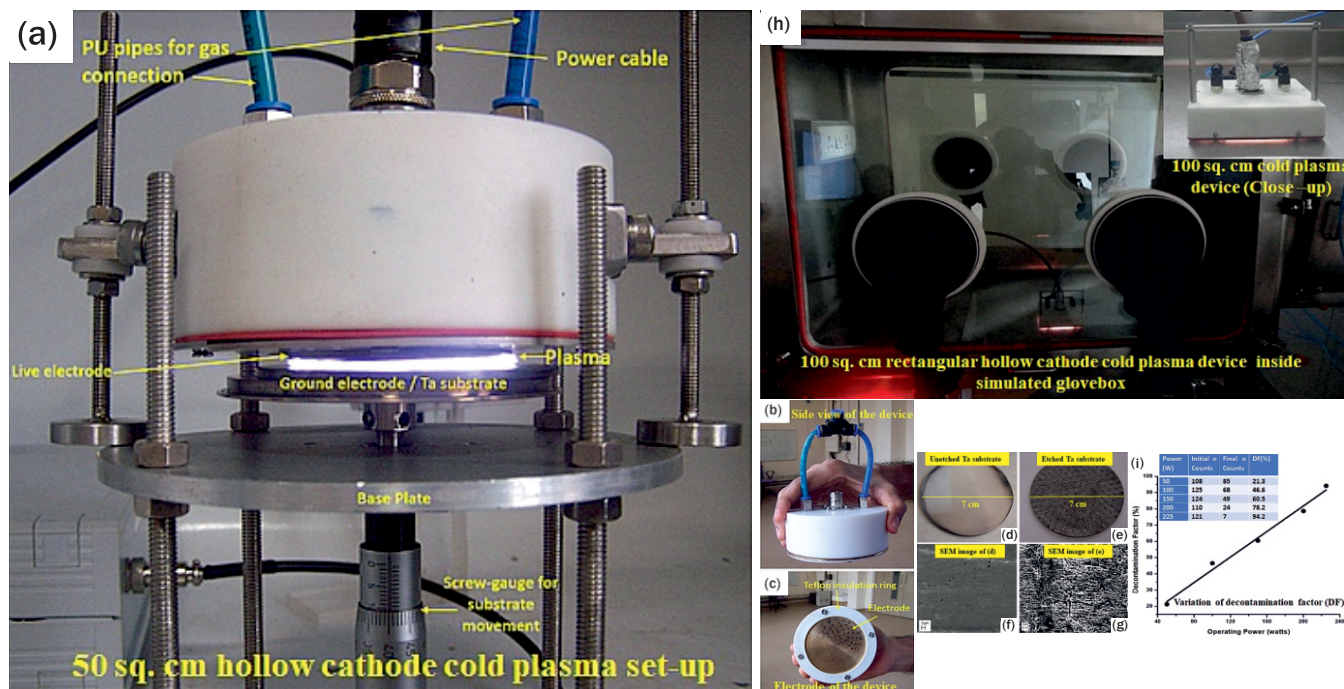
Distinct metal-specific trends were observed. Titanium clusters readily form extended nitride series (TiN_n), whereas vanadium and iron clusters predominantly yield mononitrides, with size-dependent efficiency of NH_3 dehydrogenation. Cobalt clusters exhibit limited reactivity, primarily through ammonia adsorption and partial dehydrogenation. In contrast, nickel clusters show unique behavior—forming stable solvated nitride/imide complexes and even releasing molecular hydrogen (H_2) via Ni^+ hydrogenation pathways. Theoretical calculations validated the experimental findings, highlighting the role of cluster size, charge state, and electronic structure in governing N–H bond activation and hydrogen evolution.

Reference:

J. Phys. Chem. A (2025), <https://doi.org/10.1021/acs.jpca.5c04459>

Cold Plasma Etching Tech for Solid Radioactive Waste Mitigation

From Laboratory Demonstration to Potential Glove box-Scale Deployment



Rajib Kar^{1,2*}, R. L. Bhardwaj¹, J. P. Nilaya^{1,2}, M. L. Mascarenhas³

¹Laser & Plasma Technology Division, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai-400085, INDIA.

²Homi Bhabha National Institute, Anushakti Nagar, Mumbai-400094, INDIA.

³Beam technology Development Group, Bhabha Atomic Research Centre (BARC), Trombay, Mumbai-400085, INDIA.

*E-mail for Correspondence: rajibkar@barc.gov.in

The APPJ device has been upgraded to a 100 cm² rectangular version that can be easily manoeuvred on the surface to be decontaminated. The technology holds strong promise for future applications in safe radioactive waste decontamination and disposal.

Over the past several years, the Laser & Plasma Technology Division, BARC has been engaged in the development of a cold plasma-based chemical etching technique for safe and effective decontamination of radioactive surfaces. The approach uses cold atmospheric pressure plasma generated from optimized mixtures of Ar, He, CF₄, and O. Dissociation of CF₄ in the plasma yields reactive fluorine species that convert actinides like U and Pu into volatile hexafluorides, enabling efficient surface decontamination. Our initial success was reported in a study (*Environmental Technology & Innovation*, 12 (2018), 219-229), where a 2.45 GHz microwave APPJ device demonstrated up to 94% removal of synthetic Pu contamination from glovebox surfaces. Despite the high decontamination efficiency, the active plasma area was limited (2–6 mm²), prompting further research. Subsequently, a 13.56 MHz RF-based hollow cathode plasma device was developed (Figure (a)), significantly scaling up the effective treatment area to 50 cm². Extensive testing on tantalum (a Pu surrogate) and synthetic U-laced stainless-steel samples confirmed the efficacy of the plasma-etched fluorination process. These results, recently published (*Journal of Nuclear Materials*, (2025,) 156039), showed over 94% decontamination and highlighted the critical role of oxygen in stabilizing plasma and aiding etching.

We have now upgraded the device to a 100 cm² rectangular version (Figure (h)) that can be easily manoeuvred on the surface to be decontaminated. Further modifications in the device and its testing in active environment are being planned. This scalable, substrate-independent, and cold plasma technology holds strong promise for future applications in safe radioactive waste decontamination and disposal.



On India's Growing Strengths...

India has become a global innovation powerhouse with over 100 unicorns. It is the 3rd largest startup ecosystem in the world with about a billion international internet subscribers. India's digital economy is booming. Artificial intelligence, Machine learning, Blockchain and Industry 4.0 are no longer buzzwords; they are all a reality. Digital India has connected hundreds of millions on platforms such as UPI, processed over 185 billion transactions during 2024-25. Our digital public infrastructure is admired globally and it serves as the backbone of our inclusive economic model. Many of you must have heard about it. With the click of a button, the amount of assistance is transferred to about 8 crore farmers instantaneously. This is the

On India's Climate Commitments...

India aims to install 500 GWe of non-fossil fuel capacity by 2030. We have launched the National Green Hydrogen mission. We are also co-founder of the International Solar Alliance and the Global Biofuel Alliance. Clean tech, green finance, electric vehicles, carbon trading and circular economy practices will all demand trained innovative minds where all of you (BARC) can play an important role.

Reform Measures in Nuclear Energy Sector...

Atomic energy sector can play a significant role in our clean energy initiatives and energy security. The Budget 2025-26 suggests a Nuclear Energy Mission for Viksit Bharat. Development of at least 100 GW of nuclear energy by 2047 is essential for our energy transition efforts. For achieving (this goal), both public and private sectors need to take major initiatives. Amendments to the Atomic Energy Act and the Civil Liabilities for Nuclear Damage Act will be taken up because there were some obstacles in the form of our legal provisions for private sector to participate in our nuclear energy sector. So those will be removed. It has been announced in the budget and the work is going on.

'High hopes from nuclear energy as a source of clean and sustainable power'

Dr. Pramod Kumar Mishra said in his speech during the Graduation Function of 68th Batch (OCES-2024) of BARC Training School

On Nuclear Technology Playing a Pivotal Role...

The nuclear research program will become very crucial and institutions such as BARC will play a much greater role in our strategic aspect. India's nuclear program is a matter of pride for all of us. It proved to the world that India's scientific minds can deliver on cutting edge science and technology. India had to chart its own distinct path in its nuclear program in the face of adverse external situation. Over a period of time, our program has gained respect in geopolitical and scientific communities across the world. India's nuclear agreements with several countries beginning with the agreement with the USA, the NSG waiver for our program and our participation in the ITER are some of the testimonies of the high regard that our program enjoys across the world. There are high hopes from nuclear energy as a source of clean and sustainable power. We need to capitalize on these opportunities.

On Making Nuclear Energy the Preferred Energy Option...

Nuclear energy projects are capital intensive, which affects their commercial viability if those projects are not completed on time. We can bring down project cost and tariff through access to low-cost credit, reducing operational cost and leveraging capabilities of the private sector. I am sure your (BARC) research will play an important part in reducing cost of nuclear energy so as to make it the preferred energy option. As it is well known, safety aspects of atomic energy require complete commitment as we expand nuclear energy through private sector participation and captive power plants. We also need to ensure that there is a high level of confidence in the minds of the people about safety standards of our nuclear projects.

There are high hopes from nuclear energy as a source of clean and sustainable power... The criticality of safety aspect will be very vital and we need to revisit our whole mechanisms and undertake further research on the subject... We also need to ensure that there is a high level of confidence in the minds of the people about safety standards of our nuclear projects.



A group photograph of meritorious officers who graduated from OCES-2024 program of BARC Training School.

Wishlist for a Successful Scientific Career

While extending his heartfelt good wishes to the bright and aspiring scientific officers (250 in total), who passed out of OCES-2024 program, Dr. P.K. Mishra shared an inspiring wish list for them - a vision meant to guide, motivate, and empower their journey ahead.

Embrace the spirit of lifelong learning

Embrace change as an opportunity for growth

Cultivate openness of mind, mutual respect and humility



Photos in this page courtesy of BARC Trombay and M/s. TEMA India Pvt. Ltd.



COLUMN SECTION ACTIVATION & PERFORMANCE TESTING AREA



Nuclear Power Expansion gets BARC's Heavy Water Fillip!

Private sector starts rolling out high-quality distillation columns deployed in heavy water upgradation operations of nuclear power plants based on BARC technology know-how

K.T. Shenoy, K. Bhanja, S.K. Bhattacharya, R. Bhattacharyya

Chemical Engineering Group

Bhabha Atomic Research Centre, Trombay, Mumbai-400085, INDIA

Hheavy water (D_2O) is used as moderator and coolant of all Pressurized Heavy Water Nuclear Reactors (PHWRs). Deuterium content of heavy water must be more than 99.85% (rest being normal water, H_2O) for it to be used in the nuclear reactor. During reactor operation, deuterium content in heavy water may come down (called lean heavy water), which will affect the neutron economy and thereby the power generated. Hence, heavy water needs to be withdrawn from reactor and purified (up-graded) and recycled to the reactor. The process technology adopted for this purpose is *distillation* of lean heavy water.

Distillation process is the workhorse for upgradation of liquid mixtures like lean heavy water which exploits the minor difference in volatility of D_2O and H_2O , their normal boiling points at atmospheric pressure being 373 K and 374.4 K, respectively. Industrially, this is carried out in tall distillation columns containing internals which increase the contact between vapour going upwards and the liquid going downwards. Based on the extensive study carried out earlier in BARC's Heavy Water Division (HWD), a high efficiency structured packing using phosphor bronze wire mesh was developed for this application. This wire mesh is arranged in parallel strips with oblique corrugation, assembled vertically in the form of cylindrical cartridge of 150 mm thickness, machined and cleaned before placing inside the distillation tower. These packings provide a huge mass transfer surface within a very small volume (about $700 \text{ m}^2/\text{m}^3$). Further, surface activation of the packing was developed for increasing the wettability of packing material. Thus, the packing offers twin benefits of high surface area with low pressure drop for fluid flow; this, in turn, reduce the distillation tower height and the power consumption.

Distillation towers used for upgradation of lean heavy water in PHWRs have been optimized with modular sections of cylindrical stainless-steel columns of diameter of 1.05 m and height of 3.2 m, packed with phosphor bronze packing modules. Each packing module is ~ 150 mm thick and 17 such modules are filled in each column section. Very high efficiency and low

pressure drop collector-distributor system is also developed, which are placed at the top of each column sections for redistribution of water. In typical applications, 14 such column sections are placed vertically one above another to form the complete distillation column with total height of about 50 m, including additional tower accessories.

Nearly 30 such columns have already been manufactured and supplied by HWD and they are in successful operation in India today at various DAE establishments, including Heavy Water Board and Nuclear Power Corporation of India Limited (NPCIL). With over 40 years of experience in indigenous design, manufacture, testing and deployment of these packed distillation columns as well as long term reliable performance in critical applications of the nuclear industry that matches international performance standards. Thus, BARC has truly embodied the "Make in India" philosophy of self-reliance, by developing import substitutes even for challenging process and manufacturing technologies.

In order to support the fleet mode procurement policy to accelerate nuclear power deployment in India, it was decided to pass on this know-how to the Indian industry, to enable them to contribute more meaningfully towards supporting and accelerating the growth of installed nuclear power capacity in India. The full technical know-how was formally shared with six industries through the technology transfer mechanism.

Out of the 6 Indian industries which have acquired this technology through licensing, M/s. TEMA India Pvt. Ltd. has been selected by NPCIL after detailed technical and financial evaluation to supply the first 12 of the columns required for its upcoming projects. Major challenge for the vendor development

Photo feature from the left hand top side;

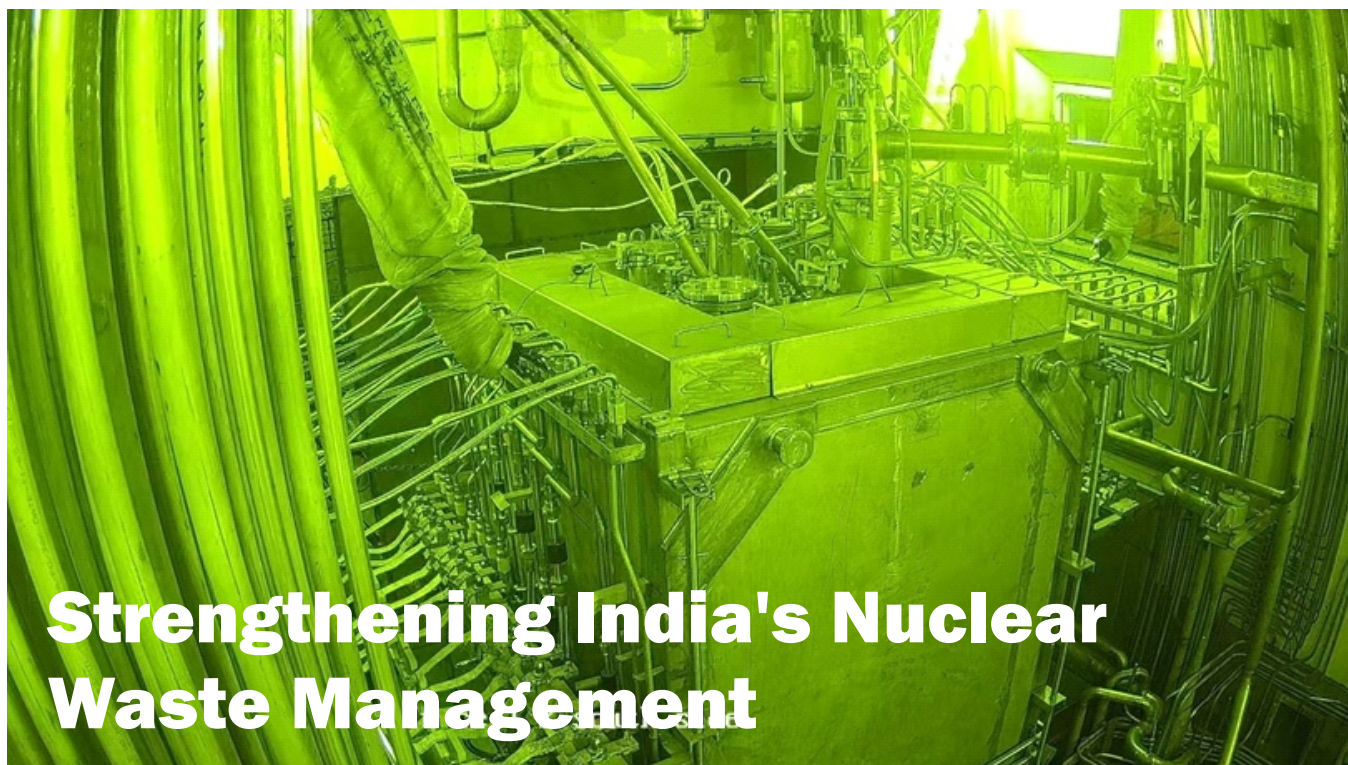
Flag-off ceremony at TEMA - Optical Alignment Set up - Activation Set up - Single Set up Machining - TEMA Test Facility - Acid Alkali Set up - Column section being filled with packing modules - Column performance test facility.

and establish manufacturing facility at vendor's site is its intricacy and strict quality control to be followed during fabrication, assembly and testing. High precision machining, laser alignment, lip seal joints etc. require very tight quality control. Machining and other infrastructure were created at the vendor's place with required technical support and hand holding from BARC. One of the major concerns is skilled and experienced manpower, which is essential to avoid rejection as it costs time and leads to material wastage. This was addressed by giving training to the vendor's manpower at the facility available in BARC.

With the support of BARC and NPCIL, M/s. TEMA has developed a state-of-the-art manufacturing center at Achhad, Palghar, Maharashtra. At this TEMA facility, BARC's technology has been very successfully commercialized, in a way that is capable of meeting the stringent requirements of NPCIL. This is the first of its kind manufacturing facility in India for production of distillation columns in nuclear service. On 26th July 2025, the first qualified consignment of the distillation columns was flagged off from Achhad to NPCIL project site, RAPP 7 and 8, Rawatbhata, in presence of BARC and NPCIL officers. This development may also be cited as a very significant example of the Public – Private Partnerships in domestic manufacturer of components for hi-tech sectors that are necessary for India's technological progress.

As India is expanding its nuclear power program to 22 GW by 2032 and 100 GW by the year 2047, from nearly 9 GW of present capacity with PHWRs as its backbone, it is essential to gear up to meet upcoming huge demand of heavy water which is produced by HWB. Such distillation columns are used during heavy water production for enrichment from about 15% D₂O (produced through various chemical exchange routes) to moderator grade of >99.8%. Thus, there is huge potential for deployment in nuclear industry. At present this technology is available with very few global entities, which necessitates indigenization for self-reliance and GOI's 'Aatmanirbhar Bharat' goal. These in-house developed columns have shown excellent and reliable performance, thus establishing their merit as an economical import substitute technology.

The present technology is tailor made for heavy water upgradation by distillation, which is specific to nuclear industry only. However, similar technology with other material of construction, like stainless steel instead of phosphor bronze material will have many industrial applications for separation processes in petrochemical and pharmaceutical applications. BARC is working on to popularize high efficiency column packing fabrication technology for energy efficient and cost-effective processing of difficult to separate solutions & customization to specific industry through incubation route.



Strengthening India's Nuclear Waste Management

The Joule Heated Ceramic Melter (JHCM) in operation at AVS Annex Facility in NRB Tarapur.

Nuclear Recycle Board, BARC hot commissioned the AVS Annex Vitrification Facility at Tarapur, advancing sustainability, strategic capabilities and self-reliance in nuclear waste management plant operations

By Subrat Kaushik* and K.S. Vasudevan
Nuclear Recycle Board, BARC

India's nuclear power programme emphasizes fuel reprocessing or the Back-End Fuel Cycle to ensure both energy sustainability and safe management of nuclear waste. A cornerstone of this effort is vitrification of high-level waste (HLW), carried out in specialized facilities equipped with Joule Heated Ceramic Melter (JHCM) systems. Operating in extreme high-temperature and corrosive conditions, these plants reflect advanced engineering capabilities while opening avenues for innovation in materials development-cum-engineering and safe operational practices.

Vitrification Process and Waste Conditioning

The vitrification process immobilizes HLW in glass matrices, offering safe and long-term containment. The newly commissioned AVS Annex Facility at Nuclear Recycle Board Tarapur enhances this effort with two key units: 1. The Melter Cell which is built on a pioneering roll-in roll-out design (first-of-its-kind in nuclear waste management operations) and a 2. Decommissioning Cell which enables safe melter replacement and dismantling operations.

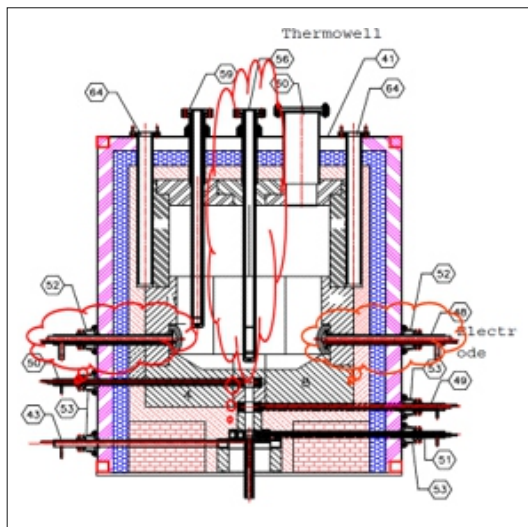
In a recent development, the AVS Annex Facility began hot commissioning in June 2025 and has the capacity to treat HLW from PREFRE-2 at Tarapur. It is specifically designed to handle HLW resulting from the reprocessing of spent PHWR reactor fuel averaging 6,700 MWD/ton burn-up of Uranium from fuel cooled for more than three years.

Engineering Challenges and Material Innovation

The operational life of JHCM is primarily limited by degradation of heating elements and internal components, exposed to harsh conditions of high radiation, continuous corrosive attack, and sustained temperatures upwards of 950°C. To address this, a new material, UNS N06690, was developed locally through collaboration between MIDHANI, Nuclear Fuel Complex, and NRB. The key components of JHCMS are now mostly fabricated from UNS N06690 billets, thereby nullifying the reliance on imports.

Key components such as electrodes, thermowells, freeze valves, and feed pipes are manufactured from UNS N06690 and thoroughly qualified for service. This material development represents a strategic technological

*Author for Correspondence: Subrat Kaushik
E-mail: subratk@tifr.res.in

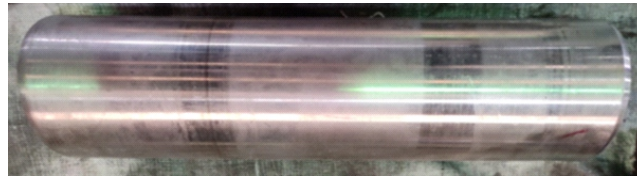


The schematic of Joule Heated Ceramic Melter (JHCM). The operational life of JHCM is primarily limited by degradation of heating elements and internal components, exposed to harsh conditions of high radiation, continuous corrosive attack, and sustained temperatures upwards of 950°C.

achievement, ensuring self-reliance and long-term operability of melters in India's backend fuel cycle programme.

Advanced Control and Power Systems

The AVS Annex incorporates modern SCADA and PLC-based systems for remote monitoring and control, minimizing worker exposure to radiation while enhancing operational efficiency. To support uninterrupted operations and ensure safe shutdown, a centralized electrical substation (TWMP



The key components of JHCMs are now mostly fabricated from UNS N06690 billets (in picture), thereby nullifying the reliance on imports.

Substation) has also been commissioned. These advanced systems guarantee that operational parameters remain within safe limits under all conditions.

Strategic Significance of AVS Annex

The indigenous development of UNS N06690, integration of cutting-edge systems, and seamless inter-agency coordination highlight the strategic importance of the AVS Annex facility. Its commissioning not only strengthens India's nuclear waste management infrastructure but also establishes a benchmark for back-end fuel cycle facilities in the future.

Authors wish to express sincere thanks to U. Dani, Former Chief Executive, Nuclear Recycle Board; present Chief Executive of NRB, Pimparkar H.R.; and Deputy Chief Executive of NRB Shri Sreekumar G. Pillai for their constant guidance and support. Authors also extend their thanks to Team of individuals at NRB for their dedication and efforts in design, installation and hot commissioning of the new facility.

Transitioning to Ever Green Revolution for enhanced National Food Security

Leading molecular geneticist, Dr. Trilochan Mohapatra, who pioneered substantial increases in domestic production of pulses and rice through research programs at the Indian Council of Agricultural Research besides prevailing over numerous other programs for new rice varieties with improved yields in tandem with advanced bio-fortification methods and crop residue management practices, was invited to BARC to deliver a talk that focused on economic, environmental, and social pillars of sustainable agriculture and India's progress toward achieving an 'Ever Green Revolution' at the popular Trombay Colloquium on 23rd July, 2025. Some of the key points of his talk have been excerpted and presented here. Presently, Dr. Mohapatra is the Chairperson of Protection of Plant Varieties & Farmers' Rights Authority (PPVFR) under the Ministry of Agriculture & Farmers Welfare, Govt. of India.

On the Significance of Green Revolution...

Highlighting the significance of Green Revolution, he stated that innovations in agriculture, driven by molecular genetics research, have enabled post-independence India to overcome the precarious "ship-to-mouth" situation in securing sufficient domestic foodgrain supplies. Continued advancements ushered in by Green Revolution, he said, later transformed India into a food surplus country and a net exporter of agri commodities. He lauded agricultural researchers, particularly highlighted the contributions of Bharat Ratna Dr. M.S. Swaminathan to India's agriculture landscape.

For a Sustainable and Remunerative Agriculture...

Emphasizing the greater need for farmers towards adapting to sustainable agriculture practices that are climate resilient and remunerative, he laid out several measures in this regard such as: Diversifying crops and cropping pattern, Conservation agriculture for improved soil health and ecology coupled with Transformation in overall farming system.

Focus on Bio-fortified Crop Varieties...

Explaining the significance of bio-fortification in crops, he highlighted key achievements such as the introduction of the improved MUKUL CR DHAN 311 variety, now widely cultivated in Assam. This variety offers 10% protein content compared to its parent variety, which has only 6-7%. Similarly, the bio-fortified AHB 1200 and HHB 311 pearl millet varieties contain significantly higher levels of iron and zinc, enhancing their nutritional value.

Key Enablers of Ever Green Revolution...

He presented several enablers that can lead to a sustained 'Ever Green Revolution' in the country, which encompass Policy Perspectives that deal with MSP and Procurement; Increased Private Partnership and Investment; Revisiting Nuclear Agriculture; Discovering New Molecules translating into enhanced local production of better pesticides and bio-stimulants; Plant Microbiomes for better yield and plant health and ecology restoration; Rhizosphere engineering; and advanced technology that contributes to smart sensors and imaging for farm deployment.

Dr. Trilochan Mohapatra

'Securing Advanced & Critical Tech edge for Viksit Bharat'

Professor Abhay Karandikar, instrumental in shaping India's telecom policy by establishing global 5G/6G standards and steering the nation's strategic vision for 6G adoption, visited BARC to deliver a talk at the popular Trombay Colloquium on 18th August, 2025. Prof. Karandikar is currently serving as Secretary to the Government of India, Department of Science and Technology, Ministry of Science & Technology. Some of the key points of his talk have been excerpted and presented here.

1 India's Global Standing in Advanced Technology...

Over the past decade, India has made remarkable progress in advanced technology and innovation. It currently ranks 39th on the Global Innovation Index, third in research publications, and third in PhD output. The country's startup ecosystem has also seen exponential growth - expanding from 11 unicorns in 2016 to 118 today - placing India third globally, with over 170,000 startups operating nationwide.

2 Focus on Critical Technologies for Vision 2047...

India ranks among the global top five in 45 of the 64 most critical technologies, including drones and robotics, cybersecurity, quantum cryptography, and quantum sensing. China leads in 57 areas, while the US dominates the remaining seven. Advanced composite materials present a significant opportunity for India, which must accelerate progress in this and other domains to achieve Vision 2047. (Source: Findings of Australian Strategic Policy Institute, published in a 2024 report)

3 National Strategy for Tech & Innovation Leadership...

Institutional reforms in tandem with efforts to bridge gaps in critical technological capabilities are being driven by greater private sector participation. Strategic initiatives such as the Anusandhan National Research Foundation - fostering collaborations between varsities and research labs - and the newly launched RDIF mechanism, which is designed to scale up private sector strengths in emerging and sunrise sectors. These are providing strong momentum to this transformation.

4 Future Paradigms...

Under the India AI Mission, the country plans to deploy nearly 30,000 GPUs to strengthen cloud computing infrastructure. India is also advancing in two key areas: Bio-engineering, through bio-foundries, biomanufacturing hubs, and precision bio-therapeutics for a sustainable future; Developing a robust Deep Tech ecosystem. Additionally, with the transition to 6G telecom services, India aims to secure at least 5% of global IPRs.



Professor Abhay Karandikar

Reports from Conferences, Theme Meetings, Seminars, and Outreach



Senior women scientific officers, Dr. Shashwati Sen (centre) and Dr. Suparna Sodaye (to her right), briefing visitors to special DAE Pavilion in the exhibition showcasing atomic energy achievements.

Women in 'STEM' empowering Viksit Bharat goal

Senior Women Scientists of BARC drive national outreach on Nuclear Energy Achievements

By Dr. Shashwati Sen and SIRD Newsletter Editorial Team

Senior scientific officers of BARC from the ranks of women represented Department of Atomic Energy (DAE) at the one-day exhibition-cum-public outreach themed Empower Women, Empower India: Viksit Bharat with Nari Shakti at Dr. Ambedkar International Centre, New Delhi on July 31, 2025.

Alongside DAE, the event saw participation of major government departments, including Indian Council of Agricultural Research, Central Council for Research in SIDDHA, Indian Council of Medical Research (ICMR) and NCERT.

Shri Lumbaram Chaudhary, Member of Parliament, Lok Sabha from Jalore, Rajasthan



A special DAE pavilion was put in place to exhibit diverse activities of BARC and various constituent units of the department with special thrust on societal applications.

took lead in organizing the program. Smt. Nimuben Jayantibhai Bambhaniya (Minister of State for Consumer Affairs, Food and Public Distribution, Govt. of Rajasthan) had been the Chief Guest. The event was also attended by several Members of Parliament, including Smt. Bijuli Kalita Medi and Smt. Kamlesh Jangde from Assam and Jharkhand, respectively. Students from various schools, an advocate from the apex court and various NGOs working for the upliftment of women too participated in the event.



Students and professionals visited the exhibition in great numbers. Centre: Senior Scientific Officer, Madhuri Shetty, guiding students understand the activities of full spectrum of Fuel Reprocessing activities in BARC.

Topics Covered

At the event, DAE showcased its strengths in nuclear technologies, radio pharmaceuticals and indigenous technologies with societal applications. Dr. Suparna Sodaye from Radio Chemistry & Isotope Group, Smt. Madhuri Shetty from Nuclear Recycle Group and Dr. Shashwati Sen from Physics Group of BARC represented the DAE delegation.

- Dr. Sodaye gave presentation on Nuclear Fuels and Radiochemistry Program covering India's three-stage nuclear power program, presenting an overview of nuclear fuel fabrication and its quality control and future plans to achieve the Amrit Kaal target for Net Zero and green energy deployment.
- Smt. Shetty spoke on Radioisotopes in healthcare sector, giving an overview of DAE's contribution in

nuclear pharmaceuticals and their application in modern diagnosis and cancer therapy.

- Dr. Sen gave an overview on the Single Crystal Activities at BARC for Research, Healthcare, Homeland Security & Energy Harvesting (Opportunities, Challenges and the Way Forward). The various developments for societal application based on single crystal for radiation detection were elaborated.

All the speakers focused on the various roles women scientists are playing in the different activities of DAE and contribution of women scientists in the department for the success of various technologies. Further, a special DAE pavilion was put in place to exhibit the diverse activities of BARC and various constituent units of the department with special thrust on societal applications. The event was well received by all and DAE's role was widely appreciated.



Industry

BARC's Nuclear

By Technology Transfer & Collaboration Division and SIRD Newsletter Editorial Team

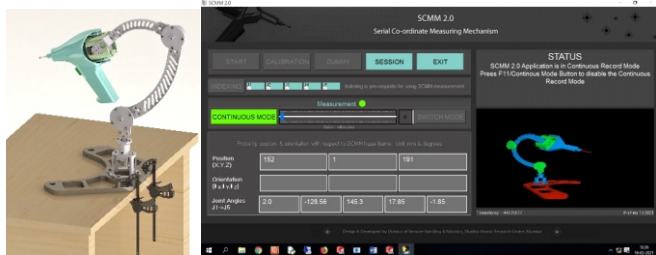
Technology Transfers

During July-August 2025 period, the Technology Transfer and Collaboration Division in BARC inked agreements with industry partners for transferring nuclear spin-off technologies with applications in agriculture, urban waste management, food preservation, engineering, water treatment among others. Key details of transferred technologies are covered here.

A Rapid Composting Technology for decomposition of dry leaves, kitchen waste and temple waste (Code:AB25NABTD) and Mass multiplication medium of Biofungicide *Trichoderma* spp. (Code:AB08NABTD) have been transferred to Solapur-based M/s. Plant Health Solutions. BARC's rapid composting technology helps in generating compost which is rich in carbon content and beneficial in enriching organic matter-depleted soils, whereas mass multiplication medium for faster growth of *Trichoderma* spp., which is an effective bio fungicide that controls fungi, promotes plant growth, improves stress tolerance, enriches soil, and eco-friendly.

The technology of Microfine Neem Biopesticide (Code: AB21NABTD) has been transferred to M/s. Bioadaptis from Punjab. Low Dose Dosimeter or ANUDOSE For Food Irradiation Application (Code: AB58FTD) technology has been transferred to Lucknow based M/s. Impartial Testing.

A host of other technologies encompassing engineering and waste management have also been transferred to the industry. These include a 100kW, 35kV Electron Beam Melting (EBM) Gun Column for Metallurgical Application (Code: EG17APPD), a Serial Coordinate Measuring Mechanism (SCMM) (Code: EG21DRHR), and the technology of Air Plasma Incinerator (Code: EG30L&PTD) (2 Nos.)



Serial Coordinate Measuring Mechanism technology, licensed to Gurgaon based M/s. QS Metrology Pvt. Ltd.



Participants at the first edition of Deep Tech Talk Series on "Harnessing the Power of Multiomics" held at DAE Convention Centre in Anushakti Nagar, Mumbai.

have been inked with M/s. Star Alucast Pvt. Ltd., (Mumbai), QS Metrology Pvt. Ltd., (Gurgaon) and Seiler Garepa India Pvt. Ltd., (Pune) & Cist Technology Solutions Pvt. Ltd., (Mumbai) respectively. Air Plasma Incinerator technology has special importance for management of waste in an environment-friendly manner.

Additionally, the technology of Hybrid Granular SBR for Wastewater Treatment (GST) (Code: EV05WSCD) has been transferred to M/s. Twarit Industries Pvt. Ltd. (Banaras) and M/s. Inovativa Waste Aid and Management Pvt. Ltd. (Goa). Further, the technology of Dissolved Oxygen (DO) Monitor (Model-1) (Code: CH32ACD) has been transferred to Pune based M/s. Primove Engineering Pvt. Ltd. In this way, BARC's nuclear spin-offs continue to achieve pan-India reach.

Advertising of New BARC Technologies BARC-DAE technologies which have significant industrial applications are regularly featured on the official webpage (<https://barc.gov.in/technologies/index.html>) of BARC. Some of the newly introduced technologies that are ready for transfer to the industry are as follows.

- **Healthcare:** Multi-contaminant Exposure Respiratory Cartridge (MERC) for Face-Mask/Respirator, developed by Chemical Engg., Group, was listed with the code MD31AMMD.
- **Cancer Care:** Novel Magneto-Liposomes for Targeted delivery of Doxorubicin and Improvement of Chemo-Radiotherapy efficacy in Cancer Patients, developed by BSG, was listed with the code AB63RB&HSD.
- **Rare Earths Recovery:** A Process for the recovery of rare earth

beckons

Spin-off Technologies

values from ankeritic ore body of Ambadongar, Gujarat, developed by Materials Group, was listed with the code CH48MinD.

AIC ANUSHAKTI

Established under the Govt. of India's flagship Atal Innovation Mission, Mumbai-headquartered AIC-ANUSHAKTI is committed to becoming a leading state-of-the-art incubation centre in deep tech, facilitating commercialization of cutting-edge technologies and supporting India's drive towards self-reliance. Some of the recent developments are as follows:

MoUs for Collaborative Activities and Start-up Incubation AIC ANUSHAKTI, HBNI inked an MoU to promote and expand deep tech entrepreneurship in the country. The MoU was inked on August 20th in the presence of Dr. A. K. Tyagi, Dean HBNI; Martin Mascarenhas, Chairman of AIC-ANUSHAKTI; and the Directors of AIC-ANUSHAKTI, Dr. P. A. Hassan and Daniel Babu. It was followed by an insightful discussion on the roadmap of activities planned at AIC-ANUSHAKTI. Further, under an MoU with PanScience Innovations - focused on promoting startup incubation activities - a total of 60 applications were received for support and 8 were shortlisted to make their pitch before a panel of experts drawn from the ranks of BARC.

Launch of Deep Tech Talk Series AIC-ANUSHAKTI launched its flagship knowledge sharing initiative, the Deep Tech Talk Series, with the first edition on "Harnessing the Power of Multiomics" delivered by Dr. Abhishek Tripathi, Co-Founder & Director (R&D Operations) of Novogene Technologies Pvt. Ltd. The event saw participation of BARC scientific community, HBNI, and college students. The inaugural address was delivered by Dr. P.A. Hassan, Associate Director, BSG and the Vote of Thanks by Daniel Babu, Head, TT&CD, BARC.

Outreach & Engagements AIC-ANUSHAKTI participated in the Incubators Conclave 2025 organized by Maharashtra State Innovation Society (MSInS) at MCMCR, Powai, for networking and ecosystem collaboration. It also visited SFIT and Thakur College as a part of focused outreach to explore collaboration opportunities and engage students in innovation and entrepreneurship activities.

AKRUTI Programme Activities

Inauguration of new AKRUTI Kendra and Agreement Signing AKRUTI Kendra – DYPACS was formally inaugurated at Dr. D.Y. Patil



AKRUTI Kendra – DYPACS inauguration function.

College of Arts, Commerce and Science near Pune in Maharashtra. Senior officials of TT&CD, NA&BTD, FTD, and DMTD present during the inauguration demonstrated to the participants - totaling 500 - the benefits of BARC nuclear spin-off technologies. The new Kendra was planned to serve as a collaborative platform to promote innovation, rural technology dissemination, and sustainable community development.

Technology Transfers & Trainings Under the auspices of the newly inaugurated AKRUTI Kendra – DYPACS an agreement was signed with M/s. Surekh Soil Testing Laboratory Pvt. Ltd. (Latur) for transfer of BARC's Soil Organic Carbon Detection Kit. Meanwhile, numerous programs viz., trainings, workshops and awareness camps were conducted/held by AKRUTI Kendra - Tarapur for widespread dissemination of BARC technologies for rural entrepreneurship.

Trainings: Sarpada Village from 23rd July 2025 to 30th July 2025 on Food technologies; Food Processing during 22-24 August; Fabrication of water purifier candles. **Workshops:** On BARC Technologies during Adivasi Diwas at TAPS Colony on August 9th.

Awareness Camps: July-August period saw programs held at Sankalp Mahila Prabhag Sangh (Atmashakti Nagar), Sanjeevani Foods (Pasthal), Sankalp Mahila Bachat Gat (Pasthal), Kosbad Village (Dahanu taluka in Palghar). Additionally, AKRUTI Kendra-SVERI participated in Pandharpur wari programme by establishing a stall which saw significant footfalls.

As on date, 12 AKRUTI Kendras are operational across the country in Andhra Pradesh, Chhattisgarh, Maharashtra, Karnataka, Kerala and West Bengal. The AKRUTI Kendra-Tarapur was established through a CSR initiative of NPCIL.

The Compass of Knowledge



Select Glimpses of Book Exhibition in Central Library, BKR&

