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One of the raw materials of the D-T fusion reaction, deuterium, is naturally available in seawater, where there is approximately one deuterium atom for every 6,000 hydrogen atoms. Whereas, the other reactant, radioactive tritium with a half life of 12.32 years is scarce in nature and has to be bred inside the reactor itself with the aid of breeding blanket systems. In the breeder blanket system, tritium is produced due to the neutron irradiation of lithium atoms in the blanket modules. The breeding blankets and their associated systems must achieve tritium-breeding self-sufficiency to ensure good power conversion efficiency in a fusion reactor. To realize tritium self-sufficiency in the reactor, it is essential to effectively recover the tritium and other hydrogen isotopologues from the breeder zones in the tritium extraction system (TES). In addition, only ~1-3 % of the fuel in the fusion reactor is burnt in the tokamak to produce energy and the remaining 97 % of the D-T fuel remain unburnt. Hence, to enable safety and effective fuel utilization, it is essential to purify and recover the unburnt fuel in the tokamak using tokamak exhaust processing (TEP) system. The system for the effective extraction of tritium from breeder blankets, recovery of tritium from unburnt fuel and purification of these streams to remove helium gas, O₂, N₂, H₂O impurities in the case of TES and hydrocarbon impurities in the TEP form the inner and outer fuel cycle of the fusion fuel cycle (FFC) system.

The removal of the trace quantities of hydrogen and its isotopologues from helium purge gas is crucial for the effective recovery of hydrogen isotopologues in the TES. One of the important subsystem of TES is the cryogenic molecular sieve bed (CMSB) system that works on the principle of molecular physisorption of hydrogen isotopologues on zeolite beds at 77.4 K [1]. Zeolite molecular sieves of Linde type A (LTA) framework are considered potential adsorbent materials for the CMSB of TES. In order to design a CMSB system for TES, adsorption data in the form of equilibrium adsorption isotherms and capacities are required. Though adsorption data is available for H₂-D₂ adsorption on zeolites, the adsorption isotherm data of hybrid isotopologues HD HT, DT, and radioactive T₂ on LTA 4A zeolites at low pressures (1-1000 Pa) and 77.4 K temperature is not available in the literature. Hence, Grand Canonical Monte Carlo (GCMC) simulations were performed in the present work using the super computing facility at IPR, ANTYA, to study the hydrogen isotopologues adsorption in the pressure and temperature ranges of operation of the CMSB of TES [2]. The simulation took 96 hours with 40 CPU cores on a single node of ANTYA.

Molecular Simulations of Low-Pressure Interaction of Hydrogen Isotopologues on Zeolites - Implications for Fusion Fuel Cycle Applications

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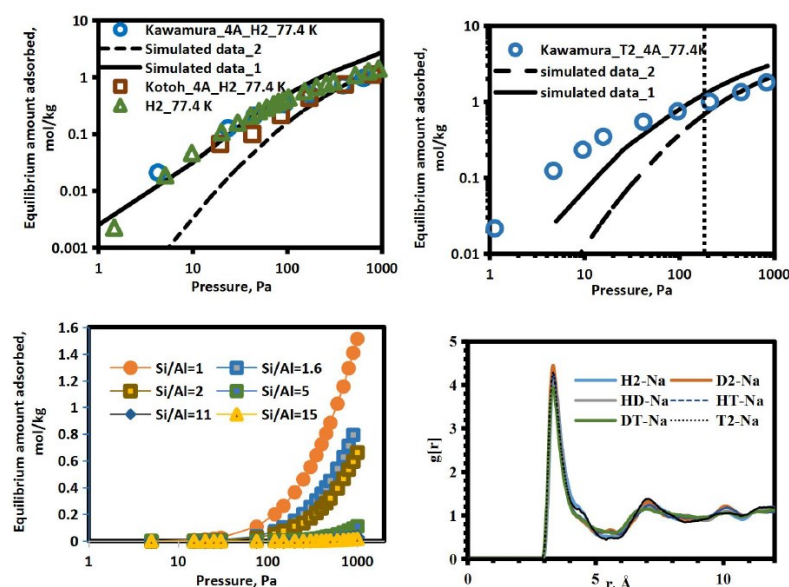
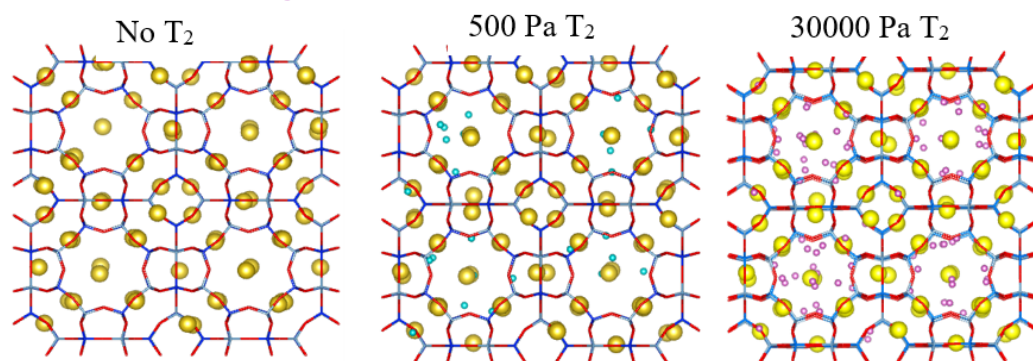


Fig. 1: (a) Snapshots of LTA4A zeolite with cation in the equilibrated positions, T₂ adsorption at 500 & 30000 Pa; Comparison of different experimental data with simulated isotherms for (b) H₂ (c) T₂ loading on LTA4A at 77.4 K (d) Effect of Si/Al ratio on equilibrium loading (e) RDFs for the hydrogen isotopologues with Na⁺ cations in LT4A zeolites for Si/Al ratio =1 simulated for P = 1-1000 Pa and T =77.4 K.

logues on zeolite beds at 77.4 K [1]. Zeolite molecular sieves of Linde type A (LTA) framework are considered potential adsorbent materials for the CMSB of TES. In order to design a CMSB system for TES, adsorption data in the form of equilibrium adsorption isotherms and capacities are required. Though adsorption data is available for H₂-D₂ adsorption on zeolites, the adsorption isotherm data of hybrid isotopologues HD HT, DT, and radioactive T₂ on LTA 4A zeolites at low pressures (1-1000 Pa) and 77.4 K temperature is not available in the literature. Hence, Grand Canonical Monte Carlo (GCMC) simulations were performed in the present work using the super computing facility at IPR, ANTYA, to study the hydrogen isotopologues adsorption in the pressure and temperature ranges of operation of the CMSB of TES [2]. The simulation took 96 hours with 40 CPU cores on a single node of ANTYA.

One of the key advantages of using **GCMC simulations** is the ability to investigate **molecular-level interactions** between hydrogen isotopologues and the internal structure of zeolites (Representative snapshot of adsorption shown in Fig. 1a). This is extremely difficult to visualize through macroscopic adsorption experiments. While experimental methods can measure overall adsorption capacity, they often cannot reveal the nature of interaction, how molecules are distributed within the pores, how strongly the adsorbates interact with specific sites, or how framework composition (like the Si/Al ratio) influences local adsorption behavior. GCMC simulations provide this microscopic insight by model-

ing individual molecule movements, orientations, and energetics within the zeolite structure. This level of detail helps researchers understand **why** certain isotopes adsorb more strongly than others and guides the rational design of adsorbents tailored for specific separation tasks in the fusion fuel cycle.

The energy function for the calculation of the potential energy in GCMC simulations for an interacting pair in the system is divided into two parts, the dispersion energy term given by the Lennard- Jones (L-J) interaction potential and the electrostatic energy term given by the columbic potential given as [2],

$$U_{ij} = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{r_{ij}} \quad (1)$$

where U_{ij} is the potential energy of interaction for the pair i-j; ε_{ij} is the depth of potential energy well; r_{ij} is the distance between the two molecules i and j; q is the point charges on the particles; ε_0 is the vacuum permittivity of free space.

The modified Feynman- Hibbs (F-H) Lennard - Jones potential is used for interactions involving hydrogen isotopes. It incorporates quantum effects to describe the adsorbate-host-cation interactions at sub-ambient temperatures. Simplifying, we get the effective potential [2] by incorporating the electrostatic term as,

$$U_{ij}^* = 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] + \frac{h^2}{24\mu_{ij}k_B T} \left[132 \frac{\sigma_{ij}^{12}}{r_{ij}^{14}} - 30 \frac{\sigma_{ij}^6}{r_{ij}^8} \right] + \frac{1}{2} \left(\frac{h^2}{24\mu_{ij}k_B T} \right)^2 \left[24024 \frac{\sigma_{ij}^{12}}{r_{ij}^{16}} - 1680 \frac{\sigma_{ij}^6}{r_{ij}^{10}} \right] + \frac{1}{4\pi\varepsilon_0} \frac{q_i q_j}{r_{ij}} \quad (2)$$

where U_{ij}^* is the F-H quantum effects corrected potential energy of interaction for the pair i-j; μ_{ij} is the reduced mass of the interacting pair, h is the Plank's constant, and $1/k_B T$ is the Boltzmann factor.

In all the simulations performed in this work, L-J interactions were truncated and shifted to 0 at a cut-off radius of 12Å. The precision of 10^{-6} is set for the long-range electrostatic interaction calculated using the Ewald summation method. The LTA zeolite framework is considered rigid, an assumption widely used and validated in several research works while studying adsorbate sizes that are small enough to pass through the rings and channels. For the generation of adsorption isotherm points, four Monte Carlo particle moves, translation, rotation, random reinsertion, and swap, were considered in the GC ensemble. For the GCMC simulations, at each pressure point, 2×10^5 equilibration steps are performed to equilibrate the system, and 5×10^5 cycles were used for the production run. The ensemble averages were calculated from block averages of 5 blocks by considering the average loading from the last 20,000 cycles. Since low-pressure adsorption isotherms are generated, the fugacity coefficient of the gas phase in the imaginary reservoir is fixed at 1. The pure component isotherms were generated for LTA4A at temperatures 77.4 K and 87.3 K and for the pressure range of 1- 1000 Pa.

The adsorption isotherms (Representative isotherm for H_2 & T_2 shown in Fig. 1b & c) indicated that the equilibrium loading capacity is larger for T_2 , followed by D_2 and H_2 at 77.4 K. In the case of hetero-nuclear isotopologues, the loading capacity is larger for DT, followed by HT and HD under the same conditions of interest. The increase in the equilibrium adsorption capacity with isotopic mass could be attributed to the reduction in the zero-point energies of the isotopologues as their molecular mass increases. The isotopic effect of Si/Al ratio (Fig. 1d) on the equilibrium loading demonstrated that the isotopic mass and the cation number induce marked variation in the equilibrium loading of the adsorbate on the adsorbent at the same temperature. The results also show that, as the Si/Al ratio decreased, the equilibrium loading of the hydrogen molecules increased. The results obtained from this work are in good agreement with our experimental results and published data in the literature (with relative average deviation (RAD) of < 30% in all the cases). The heat of adsorption of the isotopologues corroborated sufficiently with our experimental results at dilute loadings and indicated weak interactions between the adsorbate and adsorbent. The radial distribution function (Fig. 1e) for Na- H_2 interaction reveals that in addition to physisorption, the electrostatic interaction between the charge balancing cation and the quadrupolar hydrogen also contributes to adsorption. The low pressure adsorption isotherms are critical for reliable design of CMSB and have a direct implication on the recovery efficiency of the hydrogen isotopologues at the outlet of the bed. Since hydrogen is released in the radioactive HT form in the breeder blanket system and experimentation with HT is not feasible at present, the data generated from this work provides valuable information for the effective design of CMSB. The simulation method adopted also provides scope for performing high throughput screening analysis with various zeolites that are more stable and superior to LTA zeolites. Some of these may be considered potential adsorbents for CMSB in the future. In addition, analyzing the effect of the Si/Al ratio provided valuable insights that might be adopted to tailor the zeolites by functionalization them to suit specific requirements. In our future work, we would be interested in accurate force field parametrization for cationic zeolites and synthesizing metal ion-modified zeolites.

References:

- 1) V. Gayathri Devi, A. Kannan, D. Yadav, P. Dhorajiya, R. Bhattacharya and A. Sircar, Effective Cryosorption of Trace Levels of Hydrogen Isotopologues on MS 13X Zeolite: Implications for Fusion Fuel Cycle Applications, Microporous and Mesoporous Materials, 385 (2025), article 113464.
- 2) V. Gayathri Devi, A. Kannan, D. Yadav and A. Sircar, Low pressure adsorption of hydrogen isotopologues on LTA 4A zeolites - A GCMC study, Fusion Engineering and Design, 188, March (2023), article 113401

The HPC Software Stack: Spack + Conda + Singularity for Reproducible and Portable Workflows

High-Performance Computing (HPC) environments are evolving rapidly, with increasingly heterogeneous architectures, collaborative research, and demands for reproducibility and portability. HPC Users, Scientists and Engineers need robust tools to manage software complexity, ensure reproducibility, and seamlessly transition workloads across systems. In this context, a triad of tools - **Spack**, **Conda**, and **Singularity** - has emerged as a powerful, flexible software stack for modern HPC workflows.

This article explores why combining **Spack**, **Conda**, and **Singularity** forms the **HPC software stack**, and how this combination addresses the real-world needs of HPC users.

Challenges of HPC Software Management

- Different clusters use different OS versions, libraries, compilers, and scheduler systems.
- Scientific software having conflicting dependencies.
- Reproducibility difficulties when environments cannot be reconfigured.
- Containers are emerging, but adoption in HPC requires compatibility with security policies and performance requirements.

To address these issues, the combination of **Spack** for package management, **Conda** for user-level Python environments, and **Singularity** for containerization should be increasingly adopted by HPC users.

A) Spack: HPC-Centric Package Management

Spack is a flexible, open-source package manager designed specifically for HPC. Unlike traditional package managers, it supports:

- Multiple versions of packages side-by-side.
- Compiler and MPI variant selection.
- Complex dependency resolution.

Spack allows users and system administrators to tailor software stacks to specific systems while maintaining reproducibility and modularity. For example, an HPC user can use Spack to install PETSc with Intel compilers on one system and with GCC on another without conflicts, while sharing the same build recipe.

B) Conda: User-Centric Python Environment Management

Conda complements Spack by managing language-specific environments - especially in Python - at the user level, which is crucial in shared HPC environments where admin privileges are restricted.

- Manages environments in user space.
- Supports dependency resolution for data science and ML tools.
- Widely used by research communities.

Workflows involving Python tools (e.g., NumPy, Pandas, TensorFlow, Jupyter) should use conda which provides isolated environments that work seamlessly with Spack-installed lower-level libraries.

Best Practice: Use Spack for system-level libraries and scientific packages (e.g., HDF5, NetCDF), and Conda for scripting environments and notebooks.

C) Singularity: HPC-Compatible Containerization

Singularity (now known as Apptainer) enables containerization tailored for HPC:

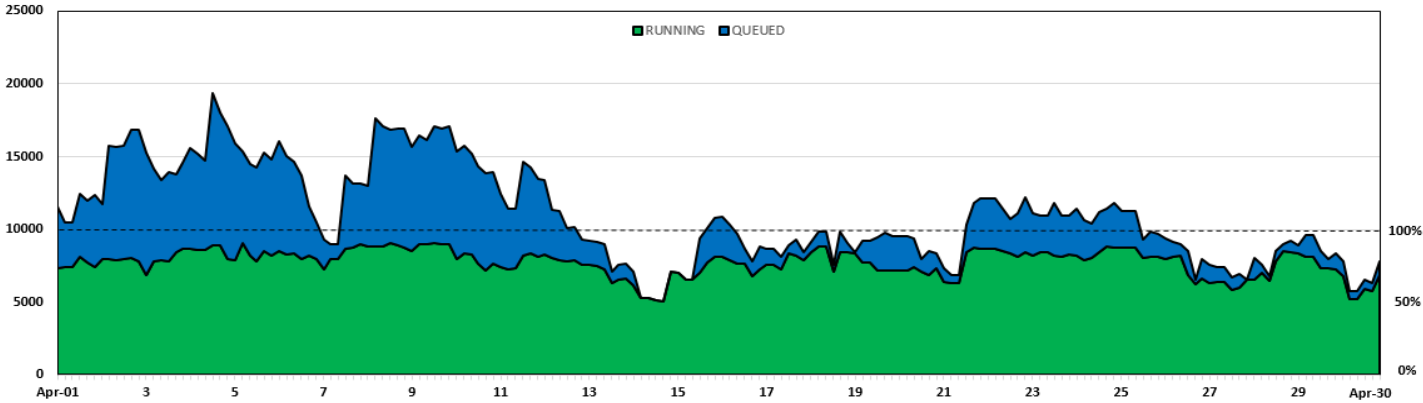
- Works without root access.
- Integrates with HPC schedulers and MPI stacks.
- Maintains file system visibility and user permissions.
- Allows portable workflows between systems.

Singularity allows packaging the entire runtime environment - including Spack and Conda setups - into a reproducible and portable container image. Prebuilt Containers from various open-source container repositories can be downloaded and used by user using singularity.

For HPC users looking to build portable, reproducible, and scalable scientific workflows, the integration of **Spack**, **Conda**, and **Singularity** represents a so called HPC software stack. This approach simplifies development, deployment, and collaboration across diverse and distributed computing environments.

ANTYA Utilization: APRIL 2025

ANTYA DAILY OBSERVED WORKLOAD



ANTYA HPC Users' Statistics
April 2025

Total Successful Jobs~ 1024

- CPU Cores [Amit Singh](#)
- GPU Cards [Shishir Biswas](#)
- Walltime [Amit Singh](#)
- Jobs [Kaushal Parikh](#)

ANTYA Usage, Updates and News

- **Scheduled Downtime:** There was no downtime of ANTYA for April 2025.
- **Job Submissions:** The highest job loads were observed in the *serialq*, *regularq*, *mediumq*, and *longq* queues, reflecting sustained user activity across multiple workloads in various queues.
- **Cluster Utilization:** The system maintained an average utilization of approximately 76.75% and peak utilisation of 90.86%.

Packages/Applications Installed: Collisional Radiative Solver (ColRadPy) module has been installed on ANTYA. \$ module load colradpy-1.0

Other Recent Work on HPC

Design and Analysis of High Voltage DC Power Supply System for Nuclear Fusion Application	Ashok Daulatram Mankani
Liquid metal MHD flow analysis in presence of a physical obstruction in a rectangular flow path	Anita Patel
Comparison of Performance Efficiency of Different Types of RF Antennas for Permanent Magnet-based Helicon Plasma Source via Finite Element Simulations	Alli Amardas
Study of edge toroidal rotation in inboard limited Aditya-U Scrape-off layer using EMC3-Eirene simulations	Arzoo Malwal
Plasma Edge Dynamics under Localized Radial Magnetic Perturbations in ADITYA-U Tokamak	Ananya Kundu
Chaotic oscillations of test electrons in capacitive discharge	RISHABH SINGH
The role of nonlinear absorption of an ECR beam for fusion plasma pre-ionization	Tulchhi Ram
Development and testing of novel hybrid CICC joint	Piyush Raj
The Effects of Intrinsic Tungsten Impurity on Unmitigated and Mitigated Major Disruptions in ITER	Trivesh Kant
Effect of Negative Magnetic Shear on Temperature Gradient Modes in ADITYA-U Tokamak	Gopal Krishna M
Reconfigurable plasma array antenna (PhD Thesis Challenge)	Manisha Jha

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