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HPC and Chemical Engineering Thermodynamics at MUT

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Chemical engineering thermodynamics encompasses not only heat engines and processes such as refrigeration and liquefaction, but also phase equilibria and rigorous yet practical models of molecular behaviour. Accurately predicting the thermophysical properties and behaviour of materials is of key importance not just from a basic science perspective, but also for the accurate modelling and design of equipment and chemical processes. This contribution provides an overview of the application of high performance computing towards chemical engineering thermodynamics research at Mangosuthu University of Technology (MUT). Simulating large systems of particles at the molecular necessarily requires significant computational effort and resources. By employing molecular simulations and computational fluid dynamics, researchers at MUT—in collaboration with scientists and engineers from other institutions such as the University of KwaZulu-Natal, Durban University of Technology, and the Nuclear Energy Corporation of South Africa—have tackled a variety of problems including biogas cleaning, clathrate hydrate stability, polymer fluorination, renewable fuel gas upgrading, cement degradation, and water pollution remediation. The importance of high performance computing to this research is outlined and the impact of selected research outputs is discussed, including notable publications which received coverage in the popular science press and research which was of immediate and practical relevance to industry.

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