The prominence of integrating Data Science with Computational Engineering is such that, it allows for a smooth transition of research in the lab to the product in the industry. In GOKUL, this is evident through some highly ambitious projects with industrial collaborations that include topics such as (i) Steel-Genome: Characterization of Steel through Machine Learning (Fig. 2), (ii) AI-driven solutions for mixed-integer problems mainly for application in a) coal blending in steel plants, b) biofuel supply chains, and c) Climate Change, and (iii) Smart Systems Biology: Screening and Ranking of drug candidates for COVID-19 prognosis through Convolutional Networks and Bio-reactor design and control through Data Science.

While each of these areas is computationally intensive with up to NP-hard complexities, the ideas from Data Science enable a real-time solution that provides a unique perspective offering multiple degrees of freedom to solve the problem intelligently. At GOKUL, we walk the path of a Computational Chemical Engineer empowered with the prowess of Data Science to explore new frontiers in Process Systems Engineering.

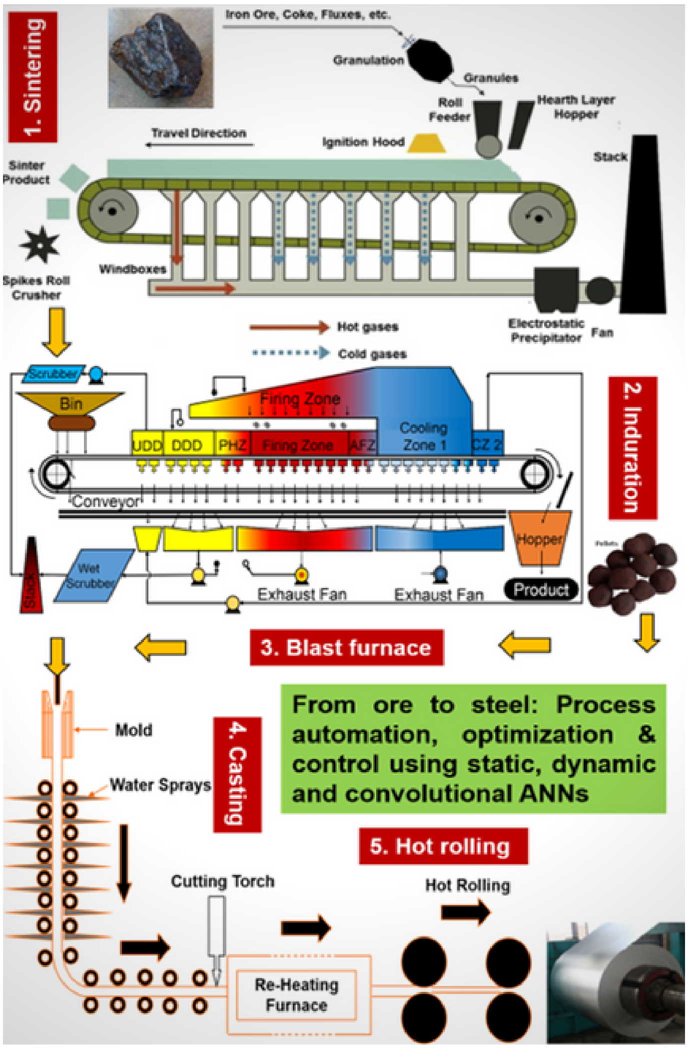

Fig. 2: From ore to steel: Process automation, optimization & control using static, dynamic & convolutional ANNs

Development and application of computational models for modelling particulate flows in Mineral Processing

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Most mineral processing unit operations involve fluid as a medium while separating the particles based on differences in their size, density, shape, and sometimes surface properties in the given slurry feed. Multiphase systems prevalent in minerals processing, usually consist of solid-solid and solid-fluid systems, such as in comminution and classification, flotation, gravity separations, dewatering, and magnetic separation, among several other unit operations. These particulate multiphase flows involve complicated physical processes and complex geometry. The majority of these flows are turbulent in nature. Tumbling mills are the first set of wet-unit operations of comminution circuits, which utilizes large amounts of water while grinding the particles to fine sizes. Dynamics of particles in the presence of water/slurry medium would behave differently than when they are treated in the dry grinding route. Understanding of internal dynamics of the charge and slurry can be of great help in energy-efficient mill design. Grinding efficiency not only depends on the tumbling mill performance but also on the recirculation load that results from the associated classifier with the circuit. Therefore, accurate prediction of classifier flow properties greatly influences the mill efficiency predictions in the given comminution circuit.

Modelling industrial cyclones (Hydrocyclone and DMC) is very challenging due to the existence of a complex flow field that is highly turbulent and varying multi-scale particles. Computational models that solve governing equations in the form of efficient multiphase and turbulence models with appropriate boundary conditions are highly desirable for accurate flow field and particle dynamics thereby affecting performance predictions.

Our group at IITH works on developing a suite of computational models ranging from computational fluid dynamics (CFD), discrete element model (DEM), and coupled CFD-DEM strategies to simulate particulate flows outlined in Fig. 1 & 2. In recent years, our focus research has been to develop and validate the multi-phase CFD models for various mineral and chemical processing units like dense medium cyclones (DMC), hydrocyclones (HC), bubble columns, fluidized beds, and flotation devices. In particular, extensive results have been obtained on the detailed multi-phase flow in DMC/HC devices in terms of air-core resolution, mean and turbulence flow field analysis, turbulent dispersion analysis w.r.to particle classification, and understanding the classification/separation mechanism, see Fig. 3.

Extensive CFD validation is also being made by using data obtained from corresponding experimental methods such as electrical resistance tomography, high-speed video imaging, gamma-ray tomography, and physical particle separation performance tests.

These multi-phase CFD models are now being utilized for design exploration to develop new efficient separation devices. We have developed an improved cyclone separator for treating high ash & high NGM coal using the GPU-based multi-phase ASM model under a sponsored project from NMDC. In an earlier DST-SERB-supported project, a novel hydrocyclone was designed for efficient beneficiation of iron ore slimes. Recently, with help of UAY-TATA Steel support, research activity is being pursued to understand multi-component particle separation under the combined action of gravity and centrifugal field within a spiral concentrator thereby designing an improved spiral concentrator for low-grade chromite ore beneficiation.

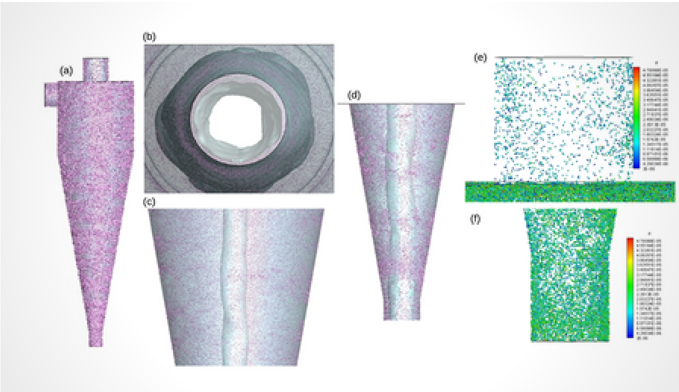
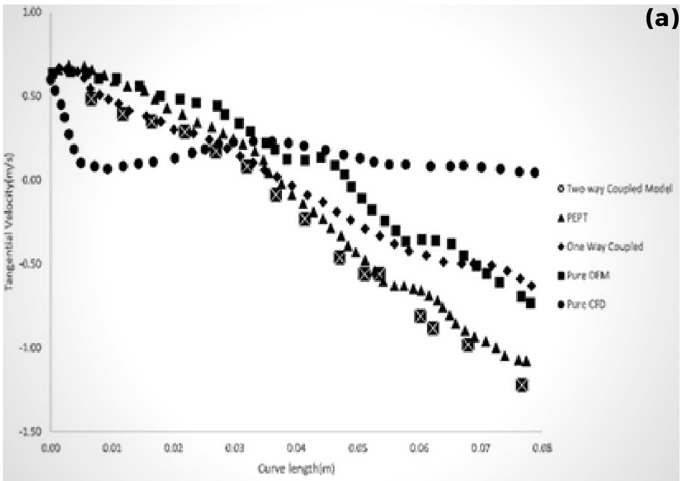


Fig. 1: Predicted particle dynamics using MPPIC-VOF approach for hydrocyclone, (a) Particle motion in the body of 3-inch cyclone, (b) High occupancy near VF, (c) Moderate concentration at a central location, (d) Swirl entrapment near spigot, (e) Smaller size particles near overflow, (f) Larger size particles near the spigot



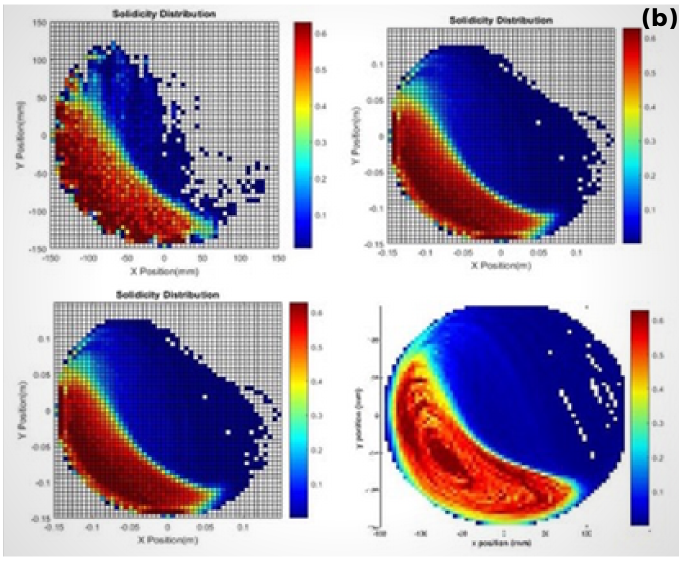


Fig. 2: (a) Comparison of tangential velocity of charge particle (obtained from EDEM) predicted by different models against PEPT data and (b) Predicted solidicity comparison. Top: (Left: DEM, Right: One-way coupling), Bottom: (Left: Two-way coupling, Right: PEPT experimental results) for the total mill volume filling of 31.25% with charge and slurry containing 20% solids.

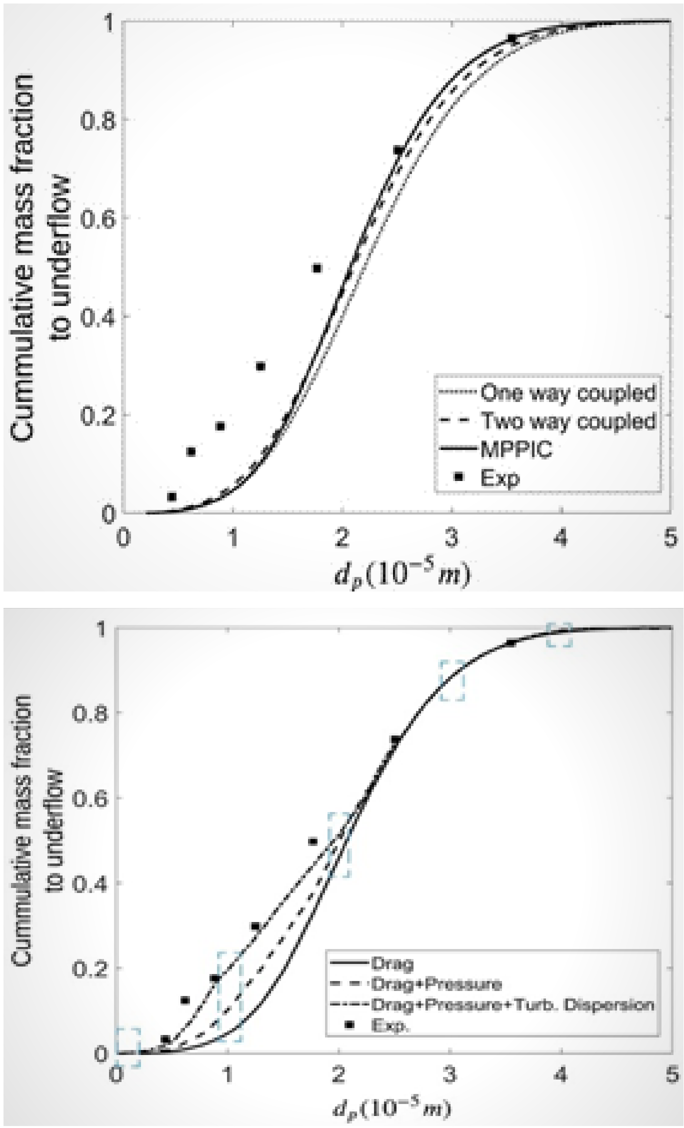


Fig. 3: Cyclone Performance comparison of different interphase forces