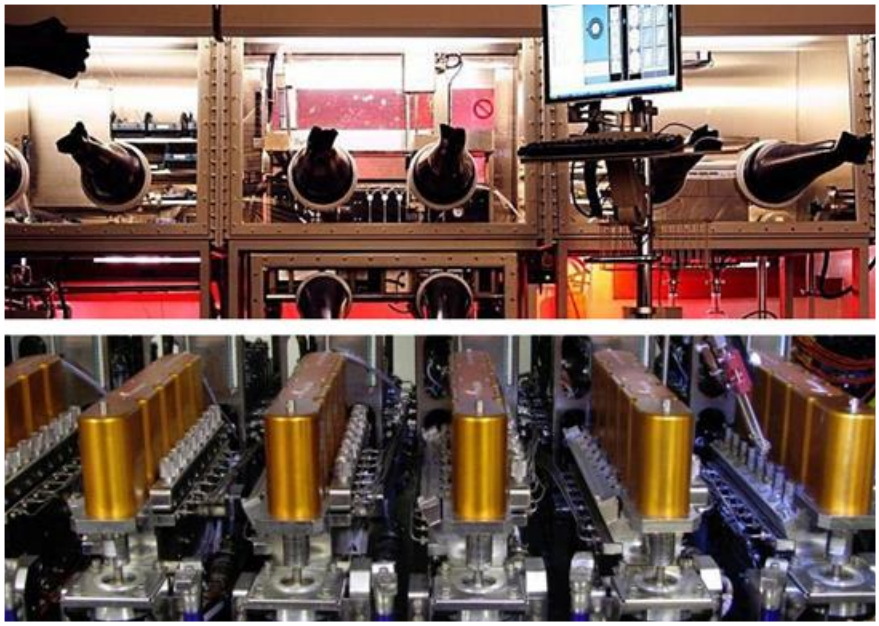
UNIVERSITÀ DEGLI STUDI DI TRIESTE

Dipartimento di Scienze Chimiche e Farmaceutiche

An Integrated HTE/ML Approach to Catalytic Coordination Polymerizations

Vincenzo Busico, Federico II University of Naples (busico@unina.it)

High Throughput Experimentation (HTE) has profoundly innovated the approach to catalytic coordination polymerizations. HTE workflows aimed at catalyst discovery and/or optimization must include advanced polymer characterization tools. Progress in recent years has been very significant, and several high-end techniques (e. g. Size Exclusion Chromatography, ^{13}C NMR spectroscopy, Crystallization Elution Fractionation, micro-capillary rheometry) can now be operated at mg scale in high-throughput mode.(1)



The approach is now being integrated with Artificial Intelligence instruments such as Machine Learning (ML), for statistical data modeling with predictive ability.(2)
Some examples of application to catalytic olefin polymerization will be illustrated and discussed.

---

(1) See e. g.: Ehm, C.; Mingione, A.; Vittoria, A.; Zaccaria, F.; Cipullo, R.; Busico, V. "High-Throughput Experimentation in Olefin Polymerization Catalysis: Facing the Challenges of Miniaturization", *Ind. Eng. Chem. Res.* **2020**, *59*, 13940−13947.
(2) See e. g.: Busico, V. et al. "ansa-Zirconocene Catalysts for Isotactic-Selective Propene Polymerization at High Temperature: A Long Story Finds a Happy Ending", *J. Am. Chem. Soc.* **2021**, *143*, 7641−7647.