Dr.Rudi Oliveira
R&D Process Safety and Scale-up Design

Optimization of a chemical reaction involves the balance of multiple parameters, such as: substrates; catalysts; reagents; solvents; concentrations; and temperatures, among other variables. Restrictions in time and costs difficult the ability to study the full range of process parameters and only a limited number of experiments are considered to find optimal conditions. Scientists typically draw upon their accumulated knowledge and available literature to identify key parameters that most significantly influence the success of a reaction at scale. To complement this Human effort, there has been significant advances in automated optimization techniques which have proven to be particularly effective, often surpassing human experts.

This presentation will demonstrate how we approached the challenge to combine some of the emerging computational tools with human expertise. Tools such as Bayesian Optimization (BO), Quantum Mechanics (QM) and Machine learning (ML) were used as part of a "virtual lab" case study to optimize a chemical reaction. The exercise was designed to resemble a real case in process chemistry as part of a drug development campaign. The performance of the different tools was compared with the path taken by different SMEs to improve yield and sustainability of the reaction, with two limitations, a threshold for impurity content and a limited number of experiments to reach the optimal conditions. The outcome of the study encouraged us to continue the integration of the computational tools without forgetting the synergism with human expertise.