ACCESSIBLE COMPUTER AIDED FORMULATION

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In civil and mechanical engineering, the design process is done almost entirely by computer. A long-held goal in formulated product design is to shift from an ad hoc labor-intensive and expensive process towards a more robust and adaptive computer aided formulation (CAF) paradigm. Recently, Formeric, have developed computational simulation methods and analytics to drive a radical change in speed of formulated product design for manufacturability and in-use performance. The goals of this work are enhanced de novo formulation design, shorter time to market, adaptive response to supply chain variability, and encouraging the adoption of formulation for sustainability. The ability to formulate virtually allows for acceleration of R&D processes, smoother development of new products, especially for high value manufacturing markets where growth arise from high R&D intensive efforts. These computer aided formulation tools are made possible by leveraging the latest cloud based platforms (e.g., AWS) methodologies. Our state-of-the-art computational models serve to advise the industrial chemist which formulations can be applied to produce products with the desired properties. In this talk we discuss the methods used in our CAF framework, highlighting successes and indicating where opportunities exist to develop the framework further. We present how the framework is being used to understand products in the fast-moving consumer goods and petrochemicals industries.