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TITLE: Physics Informed AI for CMC Applications

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ABSTRACT: While the transformative potential of artificial intelligence is broadly recognized across industries, its application within the pharmaceutical CMC space remains comparatively underutilized. A key barrier is the scarcity of experimental data typically available for individual products or development programs, which limits the effectiveness of conventional, data hungry neural network models in addressing CMC challenges such as defining robust control strategies.

Conversely, purely mechanistic models—though grounded in first principles—face their own constraints. They often struggle to capture complex physicochemical behavior using empirical kinetic relationships, and they offer limited pathways for systematic uncertainty quantification.

Physics Informed Neural Networks (PINNs) and related neural network architecures offer a promising new paradigm by integrating deep learning with fundamental physical laws. These approaches enable model development even in data sparse environments and facilitate the creation of surrogate models capable of supporting uncertainty quantification aligned with ICH Q8 principles.

In this presentation, we showcase a case study applying physics informed AI to accelerate high fidelity chromatography simulations. The resulting surrogate model substantially reduced computation time, enabling its practical use in defining an ICH Q8–compliant proven acceptable range (PAR) for regulatory submission. This example illustrates how physics informed AI can unlock new opportunities for model based CMC decision making where neither mechanistic models nor standard AI approaches alone are sufficient.