

# AI-enabled Scientific Computing Expert - Drug Product Development

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## Сводка

We are looking for an AI-enabled Scientific Computing Expert to strengthen Drug Product development capabilities within a global CMC organization. In this role, you will focus on how AI, data science, and modeling can improve decision-making in CMC, from early formulation development to commercial manufacturing. You will work in a highly interdisciplinary environment, collaborating with formulation scientists, process engineers, data scientists, and manufacturing experts to advance model-informed decision-making and embed AI-native workflows into day-to-day development activities. Rather than applying models in isolation, you will design AI-native workflows where mechanistic understanding, data-driven models, and human expertise work together.

## About the Role

### Major Accountabilities:

- You will combine process and product understanding with AI and advanced analytics to deliver decision support across the drug product lifecycle.
- The focus is on practical impact through AI-supported product development—modeling, experimentation, and knowledge management. Apply mechanistic, empirical, statistical, and hybrid (physics + machine learning) modeling approaches to support drug product formulation and process development from early lab phase through scale-up and commercialization. Translate formulation and process questions into model- and data-ready problem statements; define success criteria, assumptions, and uncertainty considerations with subject-matter experts. Use AI and advanced analytics to guide experimentation (e.g., model-based Design of Experiments, Bayesian Optimization), accelerate learning cycles, and continuously refine models as new data becomes available. Develop predictive models, digital twins, and decision-support tools for key drug product unit operations (e.g., oral solid dose manufacturing). Build end-to-end data science solutions (data preparation, exploratory analysis, modeling, validation, deployment, and lifecycle management) with a focus on transparency and reproducibility. Create clear visualizations, dashboards, and technical narratives to communicate insights and support decision making for diverse stakeholders. Contribute to automation and AI-assisted/agent-based workflows for data preparation, modeling, analysis, and reporting - improving efficiency while maintaining scientific oversight. Contribute to knowledge sharing, documentation, internal standards, and reusable modeling/AI assets within the global modeling and digital community

### Minimum Requirements

- Master's degree or PhD in chemical engineering, pharmaceutical sciences, mechanical engineering, materials science, physics, applied mathematics, statistics, data science, or a related quantitative discipline.
- Experience or strong interest in pharmaceutical development and manufacturing processes or other complex process environments. Solid understanding of transport phenomena, process science, and/or statistical modeling principles.
- Hands-on experience with programming and data analysis (primarily Python; R is a plus). Experience applying statistics, DoE, multivariate analysis, and/or machine learning in scientific or industrial settings.
- Experience using or developing machine learning models (including model evaluation and validation).
- Familiarity with AI-assisted modeling, automation, and/or agent-based workflows. Understanding of model lifecycle management, reproducibility, and deployment considerations in regulated environments.
- Experience with visualization and storytelling (e.g., dashboards or clear technical reporting).

### Desirable Requirements:

- Experience with pharmaceutical process modeling tools (e.g., PBM, gPROMS, DEM tools) and/or digital twins. Strong communication skills to explain technical concepts to non-experts and influence decisions.
- Exposure to QoD principles, PAT concepts, or regulatory-relevant modeling activities. Experience working in global matrix organizations. Ability to work with experimental and industrial datasets, including data cleaning, exploratory analysis, and uncertainty-aware interpretation including model credibility assessments according to regulatory guidelines & standard.

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