CMAC
FUTURE MANUFACTURING RESEARCH HUB

Digital Twins

Enhanced, digitally transformed
pharmaceutical manufacturing

CMAC
**FUTURE MANUFACTURING
RESEARCH HUB**

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CMAC Twins

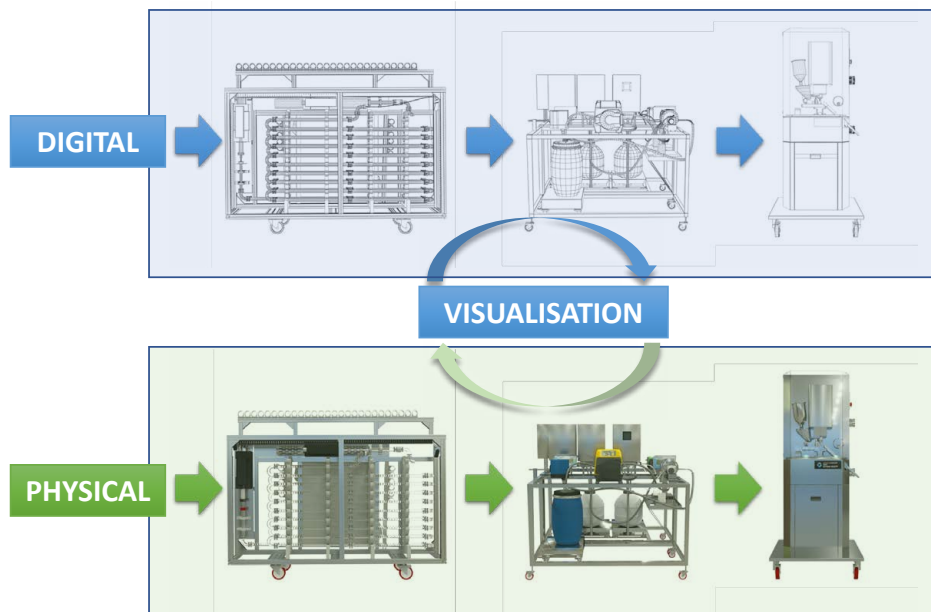*e.g. crystallise - agglomerate* → *isolate* → *compress* → *test*

Figure 1: An Example of A Digital Twin & Physical Process

The term CMAC digital twins refers to model-based simulations of transformations within unit operations or material attributes resulting from processes and characterisation tools. Data from small scale experiments/measurements are used to parameterise the models used to generate the digital twins.

The digital twins can be utilised and applied in a number of ways such as:

- To virtually design a full scale manufacturing process or individual unit ops within

- Enabling model-based experimentation to explore process conditions and determine optimal process outcomes
- Inform and prioritise "hands on" experimental approaches and key parameters to be evaluated as well as analysis of data and monitoring of systems
- Development of model-based-control systems
- Model based exploration of design changes and design optimisation for future implementations
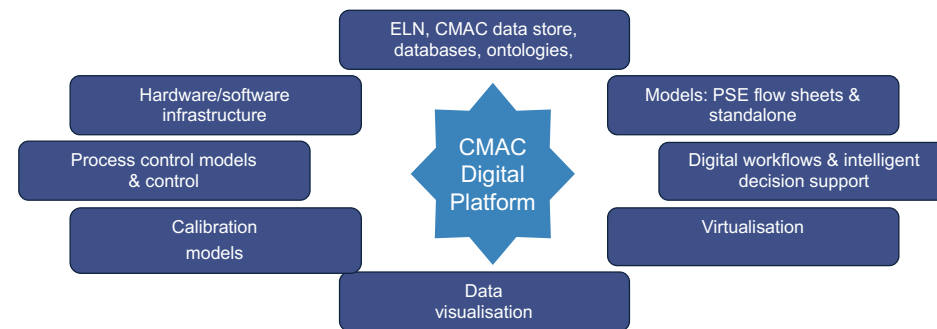- Evaluation of the impact of process on product

Figure 2: CMAC Digital Platform

CMAC has been developing an end-to-end process for manufacture of Lovastatin tablets and the digital twin is being developed alongside the physical process. Currently models for solvent screening, crystal growth, spherical agglomeration (SA), Blending and Compression and Dissolution Testing have been coupled to enable simulation of possible conditions of these integrated processes.

The models that have been used at each stage are:

Solvent Screen
- Cooling crystallisation digital workflow
- Anti-solvent digital workflow
- Application of AI-enhanced COSMOtherm solubility predictions
- SA bridging liquid selection

Crystal Growth
- Process optimisation for Crystal growth
- Computational Fluid Dynamics (CFD) models

Spherical Agglomeration
- Modified SA models

Blending and compression
- New compression model

Dissolution Testing
- At pH7 at various times
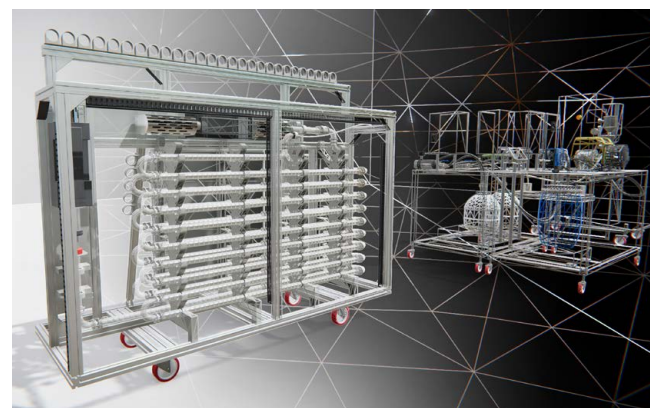
Researchers from CMAC and ARTICULAR have been working together on developing visualisation tools to support the digital twin for Lovastatin. These include AR and VR environments to interact with CMAC's rich data and more conventional dashboards that sit on top of the digital twin models. This work will then be expanded to cover the full end-to-end process and then applied to other APIs.