76c An Informatics Framework for Pharmaceutical Product Development

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Developing a pharmaceutical product formulation in a timely manner while ensuring quality is a complex process that requires systematic science based approach. Information from various categories, including properties of the drug substance and excipients, interactions between materials, unit operations, equipments etc., is gathered. Knowledge in different forms, including heuristic, decision trees, model predictions for material properties, and unit operations models, is used. Decisions regarding processing routes, choice of excipients, equipment sizing, are made based on the information and knowledge. In this work, we have developed an informatics infrastructure to assist formulation scientists in managing the information, capturing the knowledge, and providing decision support for pharmaceutical product formulation.

The foundation of this infrastructure is the modeling of the information and knowledge related to pharmaceutical product formulation. Ontology, which is the specification of a conceptualization, has been built to explicitly describe important concepts, such as material properties, unit operations, as well as meta-information of the models to describe the assumptions, information requirements and information generated from the models. Based on the domain ontology, knowledge is encoded as relations between concepts. Knowledge that incorporates workflows is modeled as guidelines. An execution engine has been developed to use various forms of knowledge to provide decision support for pharmaceutical product formulation. Methodologies and software support have been developed to integrate existing tools into this infrastructure. User interface has also been constructed to facilitate the use of the infrastructure. The functionalities of the infrastructure will be demonstrated using the development process of a legacy drug used in the treatment of multi-drug resistant tuberculosis.

The infrastructure provides a systematic approach for managing, sharing and reusing information and knowledge, resulting in considerable reduction in product development time, and increase in the quality of the formulations. Also, by providing a foundation for capturing the corporate R&D experience, the knowledge gained from one product can be applied to the development of future products.