

437b Systematic Modeling of Knowledge in Pharmaceutical Product Formulation

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Formulation of a drug product is a complex, iterative process consisting of selection of dosage form, excipients, processing routes, operating equipments and so on. At present, formulation scientists make these decisions based on the knowledge gained through years of experience. In this work, we propose to model the knowledge using formulation guidelines, which are systematically developed statements that guide decisions at various stages of formulation. The knowledge embedded in the guidelines is captured in the form of heuristics, first principles models and insights provided by experts. An ontology, which is a formal explicit specification of a shared conceptualization, is created for formulation guideline and pharmaceutical domain which define various concepts and relations relevant to formulation. A formulation guideline is created based on GLIF (GuideLine Interchange Format), which is a specification developed mainly for structured representation of clinical guidelines.

The main objective of the current project is to develop computer interpretable guidelines for product formulation in pharmaceutical industry and use them to develop an intelligent decision support system. As compared to human experts, knowledge in the form of guidelines is permanent and transferable. In a large search space, decision making is faster and more consistent. An execution engine, independent of the domain ontologies, was developed to execute the guidelines and provide the necessary decision support. In addition, an explanation component was also developed to provide the answers to reasoning behind the problem solving. Apart from helping formulation scientists in decision making, guidelines can also help them in better understanding of formulation process as well as in training.

Guidelines effectively capture the knowledge and can be used for modeling the knowledge in different domains in chemical and pharmaceutical engineering and in development of decision support systems.

Keywords: Drug formulation, knowledge modeling, formulation guidelines, intelligent system, Ontologies