27a A Holistic Approach for Modeling Information and Knowledge in Development and Operations of Chemical Processes

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During the evolution of a chemical process from product development to manufacturing different groups are assigned functions according to their expertise such as process development, process safety, process scheduling, process monitoring and so on. In the past decades, a wide variety of sophisticated tools have been developed to assist these diverse functions. In general, each tool uses information based on various forms of the knowledge the tools possesses, such as mathematics relations, heuristics etc., and generate new information. At present, the different groups of people, and the tools they use are like individual islands and with no comprehensive, integrated, environment that links these islands. This leads to a limited view of the information and knowledge, and inefficiency of sharing information as well as functionalities of these tools. This limits the supporting roles of these tools to the development and operations of chemical processes.

In this work, we have proposed a systematic approach to modeling the underlying information and various forms of knowledge. Information can either be free text, which does not conform to any predefined syntax and is poor in semantics (called unstructured information); or machine processable, which follows predefined syntax with formally defined semantics (called structured information). Ontology, which is defined as “a formal, explicit specification of a shared conceptualization”, is the foundation for modeling structured information. Ontologies for chemical process information have been created based on the existing standards which define the terminologies, and encoded in Web Ontology Language (OWL). We investigate how existing tools use the structured information modeled in ontology, and propose the best practices in ontology-driven software development. We also studied the methodology to link structured information with unstructured information, including generating structured information without interference with the workflow of the engineers, and navigating unstructured information based on the ontology. The methodologies for modeling the knowledge in quantitative and qualitative way have also been developed. The knowledge modeling is based on the ontology. So far in this project, we have concentrated on developing a prototype of the proposed holistic approach for modeling information and knowledge for chemical process development and operation. The functionalities we covered are process simulation, process safety analysis, and process scheduling.

In this paper, we present the details of the process ontology, which includes models for material properties, equipment, recipe, and chemistry. The close integration of tools based on the process ontology is demonstrated using two tools: Batches (from Batch Technologies) for process simulation, and PHASuite (from Integrated Process Solutions) for safety analysis. From process engineer's point of view, the two tools act like agents which work together seamlessly. Without intervention from the user, PHASuite uses the simulation capability of Batches to gain understanding of the process; while Batches decides parts of the process that require further detailed simulation based on the safety analysis capability of PHASuite. Process ontology also facilitates the development and integration of new tools by sharing existing information and allowing addition of new concepts when required. The proposed approach will be demonstrated using a pharmaceutical process.