
Overview of the Ontological Informatics Infrastructure for Pharmaceutical Product Development

Project Team: Venkat Venkatasubramanian
Gintaras Reklaitis
Shuo-Huan Hsu
Ankur Jain
Leaelaf Hailemariam
Pradeep Suresh
Pavan Akkisetty

*School of Chemical Engineering
Purdue University*



Overview of Informatics Challenges

- Management of a large amount of information in various formats
 - 100,000+ pages of FDA submission documentation
- Integration of different forms of knowledge and information
 - Hundreds of information repositories
- No systematic way of capturing and representing the knowledge
 - Knowledge in two forms; heuristics & mathematical models
 - Heuristic knowledge inside experts with inadequate capture
 - Mathematical knowledge tied to solvers: underlying assumptions and solutions methods hidden

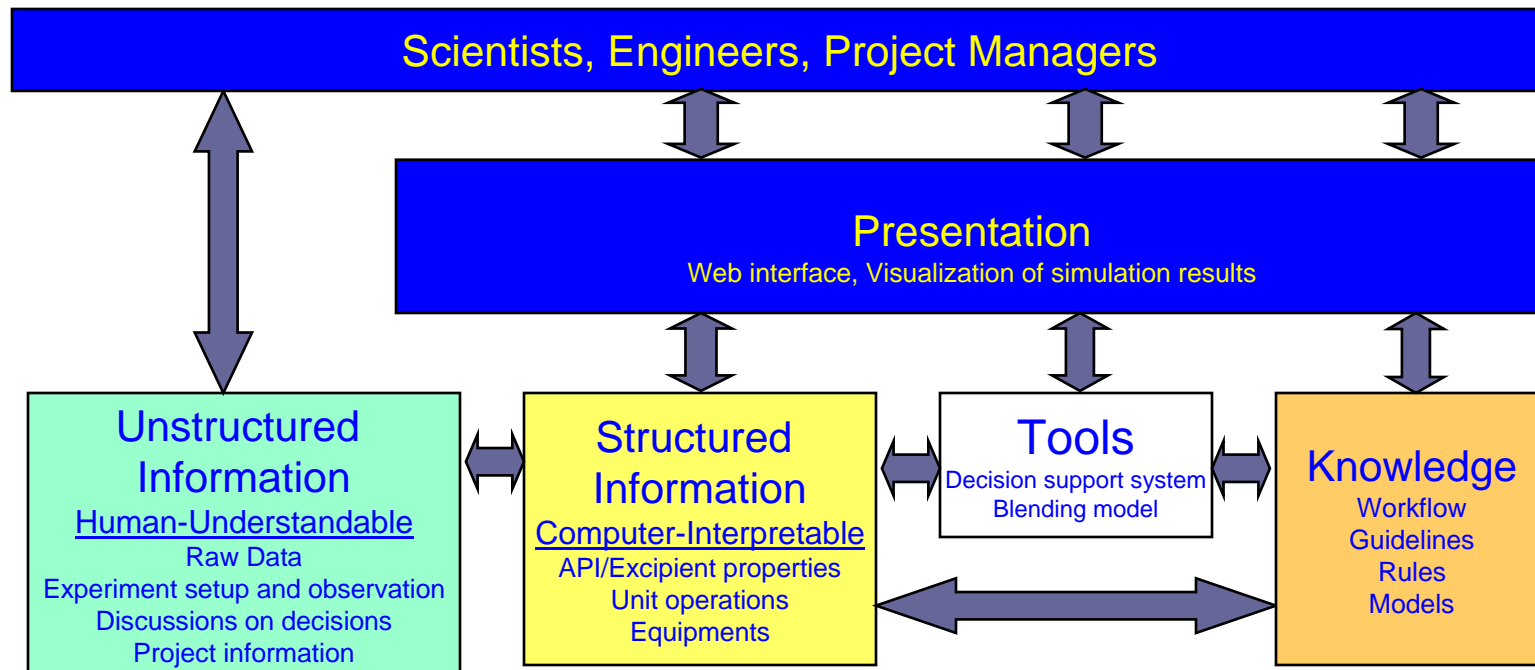
Proposed Solution

- Explicit representation of information and knowledge
 - Basis of informatics infrastructure
- Integration of knowledge and information sources through explicit information representation

- Application areas
 - Decision support for product formulation
 - Unit operation modeling
 - Real-time decision-making for design, formulation, operations, control and optimization
 - API-Excipient reaction prediction
 - Analysis of experimental steps

Ontology-based Informatics Infrastructure

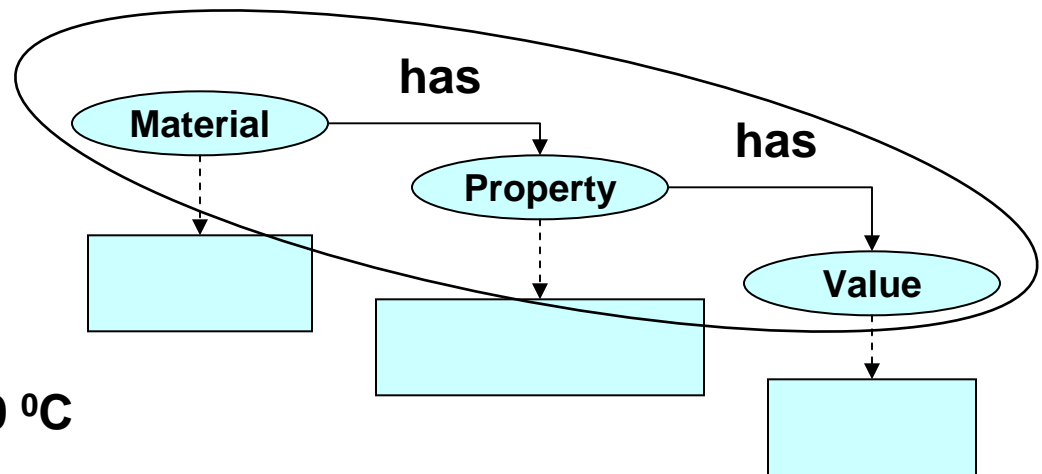
- Framework for efficient use of information and knowledge



Explicit representation of information

- A common and explicit information model required ...Ontology
- Ontology is the explicit description of domain concepts and relationships between concepts

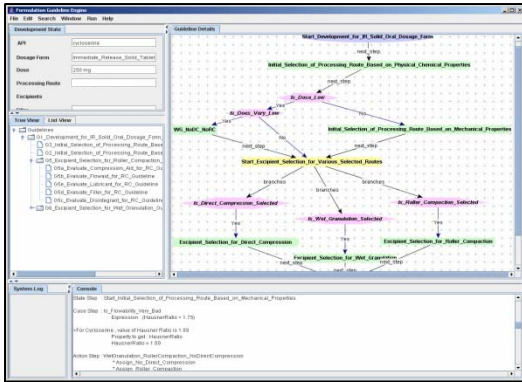
Ontology =



Water has Boiling point 100 °C

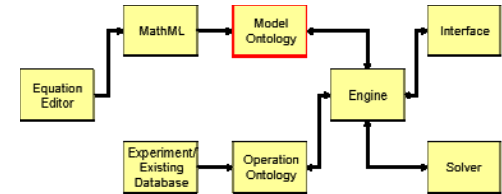
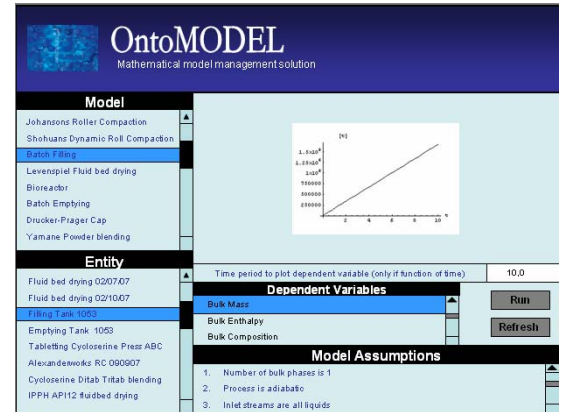
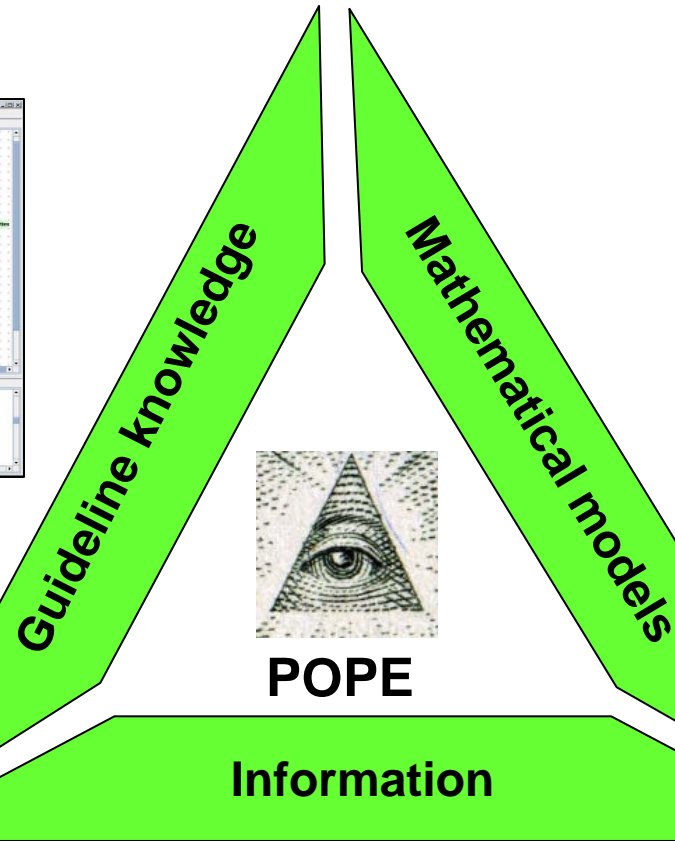
- The Purdue Ontology for Pharmaceutical Engineering (POPE) defined to describe the product development domain

POPE Components

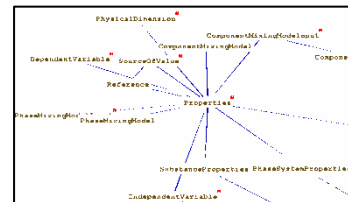
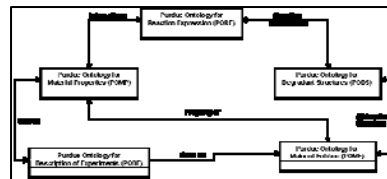


* Description of knowledge, decisions and actions

* Description of material, property, experiment, unit operation information

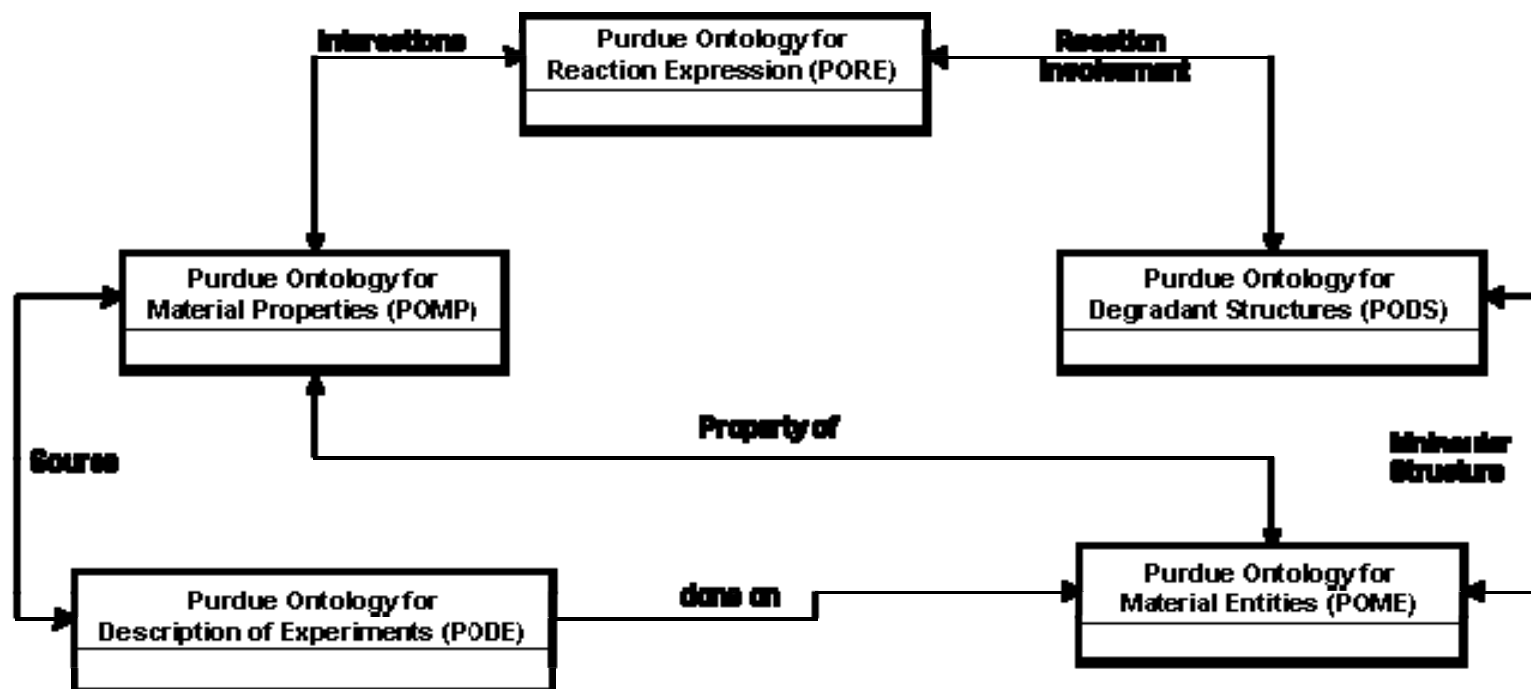


* Description of mathematical models, model use, model solution methods, assumptions



POPE – Information Representation

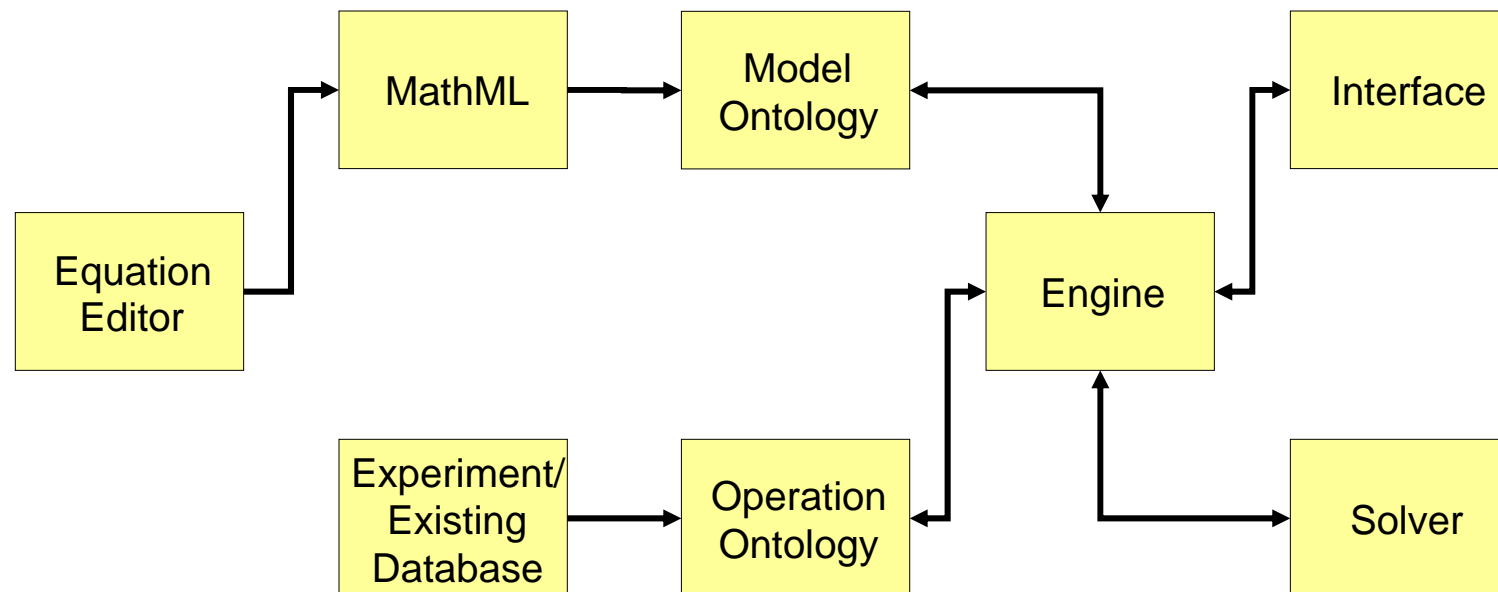
- Information representation component of POPE



- POPE-Information: repository of information entities and the connections between them

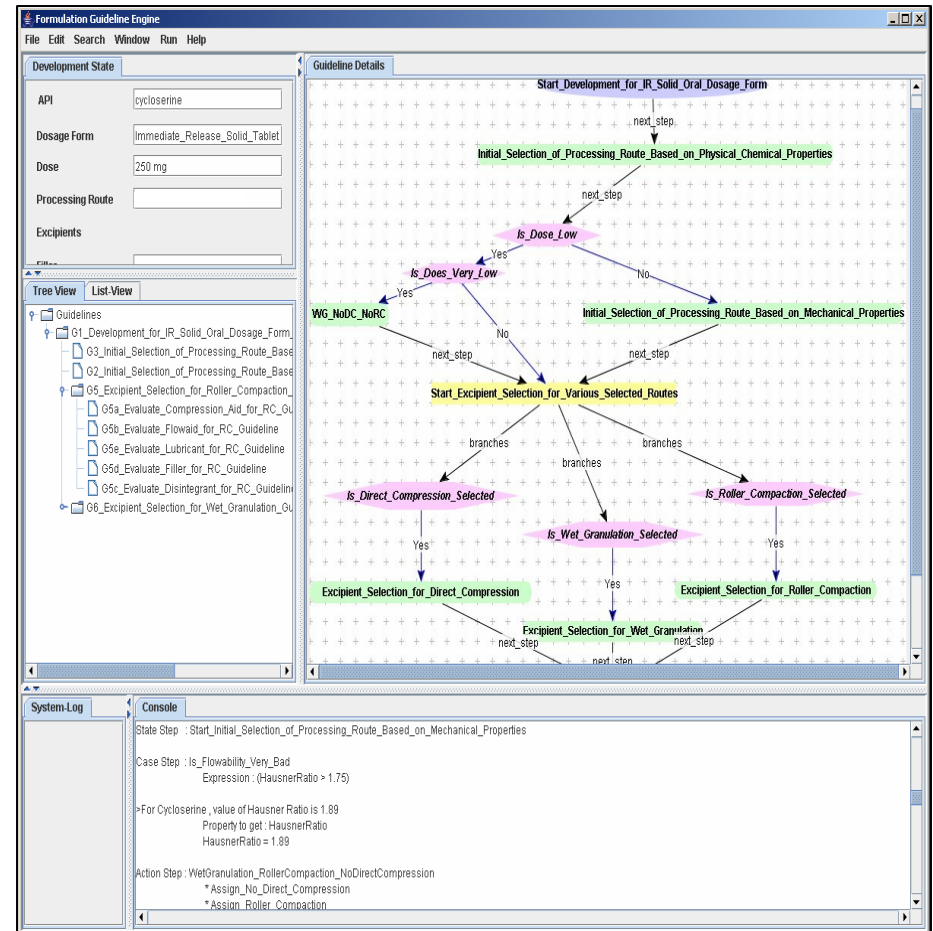
POPE – Mathematical Knowledge Representation

- Separation made between model definition and model solution
- The mathematical model and the unit operation decoupled
 - More efficient use of solvers, information



POPE – Guideline Knowledge Representation

- Knowledge represented as a set of guidelines and subguidelines
- Description of the state of product development
- Action steps to initiate subguidelines and access ontologies
- Control steps
 - synchronization
 - branch
 - Iteration
- Java Engine to execute guidelines



Interface used to perform drug product formulation