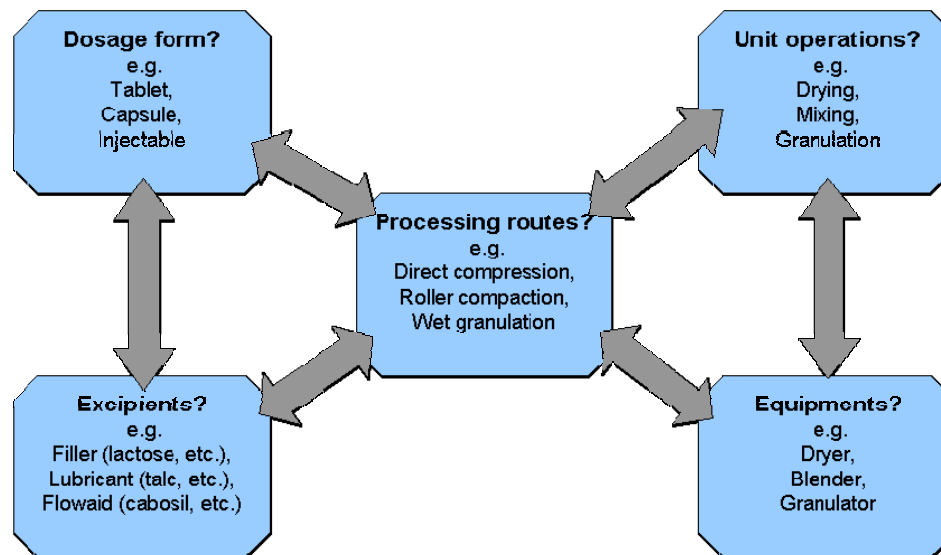

Decision support system for pharmaceutical product development

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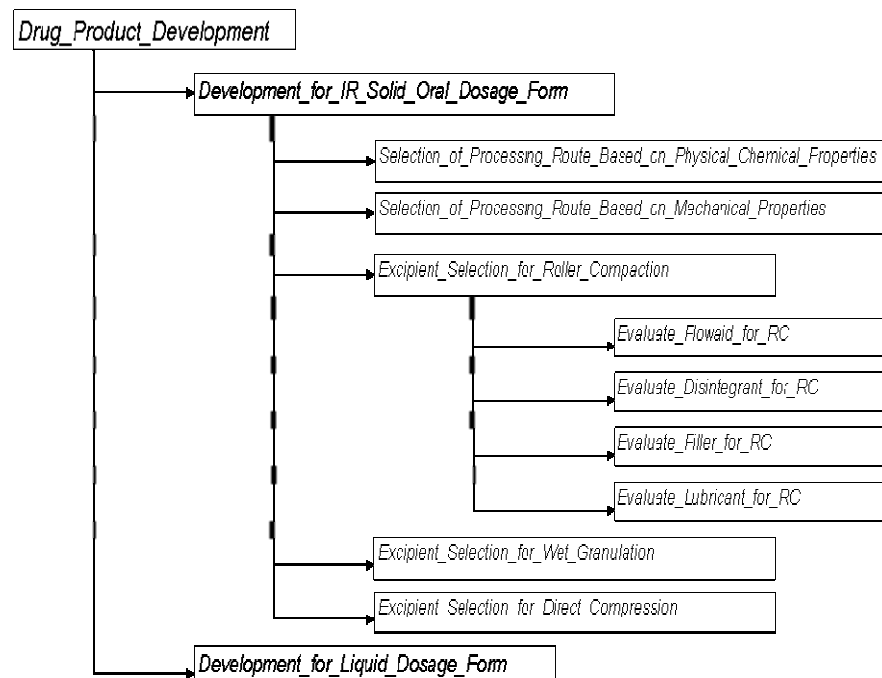
Pharmaceutical Product Development Challenges

- The life cycle of drugs includes discovery of the active compound, development of the active compound, development of the drug product before introduction to the market.
 - The manufacturing platform is a central product of product development
- Pharmaceutical product development decisions involve multiple domain and require an overarching information model



Related work

- Expert systems (containing knowledge base, inference engine, user interface)
- Limitations
 - Large collection of rules
 - Purpose of individual rule lost
 - Rule interactions rules not captured
 - Limited knowledge sharing with tools
- Proposed solution: ontology based knowledge modeling
 - Explicit representation of rules and their interactions
 - Integration with tools



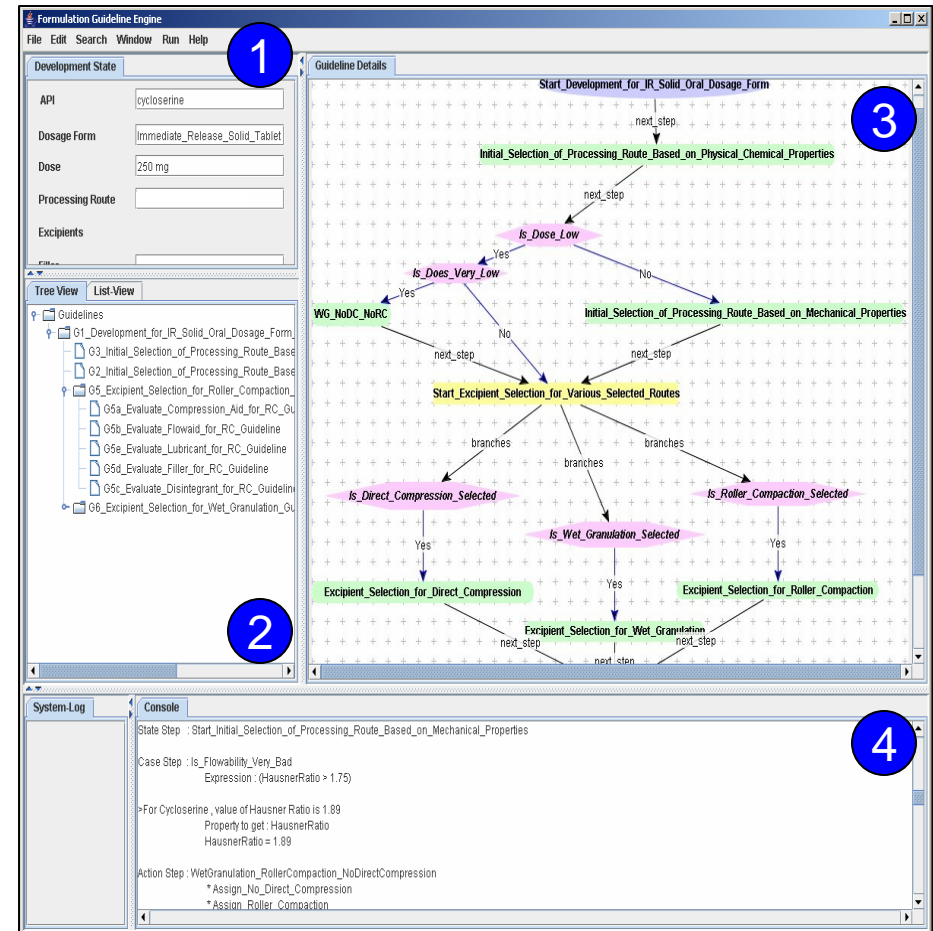
Rule hierarchy for product development

Decision Support System Overview

- Java Engine used to execute the guidelines described as ontologies

Tags:

- (1) User input
- (2) Rule hierarchy
- (3) Guideline connections
- (4) Results panel



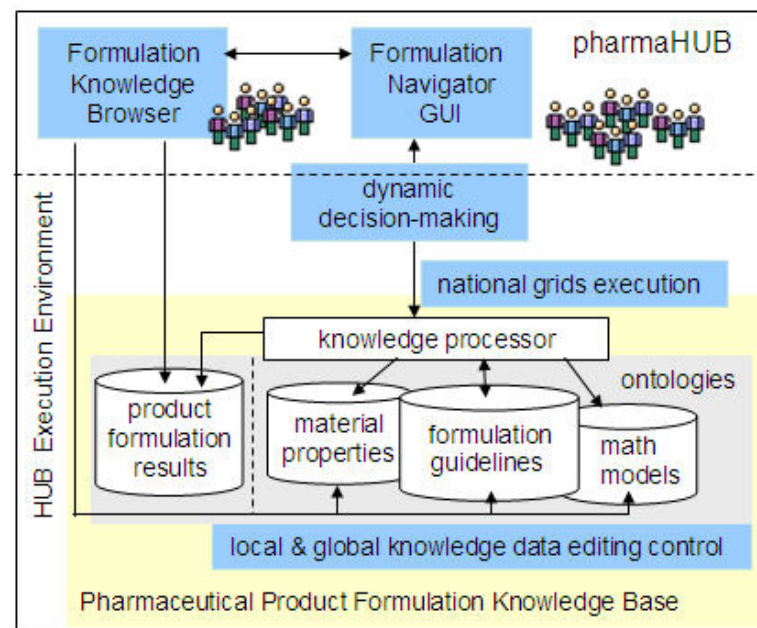
Interface used to perform drug product formulation

Pharmaceutical Informatics at the HUB

- Launch a service for shared access, browsing, and community-wide contributions to the POPE knowledge base, including

- product formulation guidelines
- decision logic & rules
- mathematical models
- materials knowledge

- Offer a graphical interface so users can visually navigate through the POPE product formulation process

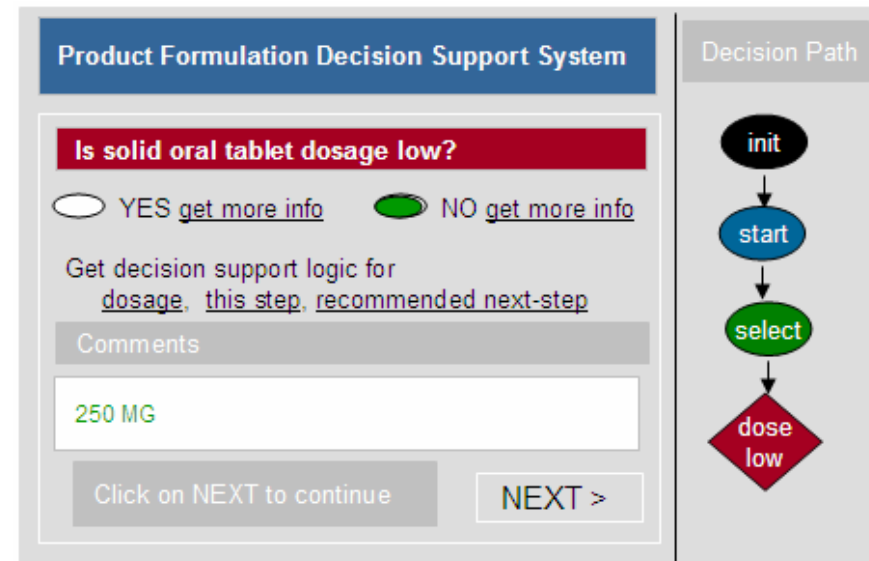


- Provide step-by-step access to all decision evaluations, material and property information, mathematical model assumptions and solutions, and other process knowledge used to generate the product formulation

Improved Decision Support for POPE

- Support interactive user control of the decision-making process – a feature that will drive “what if analysis” and alternative scenarios. Users will be able to

- respond to requests for data that will be used to determine process direction
- override recommended process decisions
- update knowledge base data during process navigation



- Record scenarios as users explore and experiment. Analyze the stored scenarios to
 - build user knowledge about optimal workflows or unexpected results
 - expand user understanding of how and why decisions are made

Advanced Decision Support Technology

- Develop enabling technologies for *general* knowledge-based decision support – beyond POPE ontology informatics
 - plug-in knowledge bases
 - fully interactive step-by-step decision-making
 - dynamic access to knowledge data during process navigation
 - information displays linked to process steps
 - local user copies of the knowledge base for what-if scenarios
 - statistical analysis and data mining across stored scenarios

- Use pharmaHUB to promote shared knowledge-building across the PES research community
 - shared community access to knowledge resources
 - growth of knowledge resources through community contributions
 - education and innovation through exploration of knowledge resources