Ontology-based Automatic Scoring Framework for Chemical Simulation System

Dong Gao, Xin Xu and Xin Ma
College of Information Science and Technology, Beijing University of Chemical Technology, P.O. Box 81, Beijing, China

Abstract: In recent years, chemical simulation systems have been widely used in operator training, chemical parameter optimization and implement of control strategy. However, it is difficult to evaluate the result of operator training, chemical parameter optimization, implement of control strategy objectively and comprehensively. In the study, an ontology-based automatic scoring framework is proposed for chemical simulation system. A scoring ontology is built in the framework for sharing and reuse of knowledge. Basing on the scoring ontology, the framework can supply evaluation of operation, performance of control loops, safety, production and consumption in the simulation system. The case study proved the efficiency, objectiveness, comprehensiveness of the framework.

Key words: Ontology, automatic scoring framework, chemical simulation system

INTRODUCTION

Petrochemical industry is one of pillar industries in China and is very important for national economy. Due to the existence of high temperature and pressure in most of petrochemical plants, it is impossible to carry out operator training using the real equipments in the plants. At the same time, as the development of technology, the plants become more and more complex and automatic. Some novel parameter optimization algorithms and control strategies are proposed. However, it is also impossible to test the algorithms and strategies in the real plants. As the development of computer technique, chemical simulation technique is proposed and widely used in operator training, chemical parameter optimization and implement of control strategy (Wu, 1999).

Firstly, the simulation systems are used for operator training. A structure of a real time dynamic simulator was proposed and the simulator was used for training in factory (Drozdowicz et al., 1987). A steady state process simulator was introduced (Melli et al., 1987). Wu et al. (1993) proposed a simulation training system in petrochemical industry. The simulation of a plant was done using ASPEN (Zheng and Furimsky, 2003). And then a novel chemical process simulator was designed for operator training (Zou et al., 2005).

As the development of simulation technique, simulation has been applied in education and research of chemical process. Hardware in loop simulation and simulation factory are proposed. A hazard, safety and control simulation platform was proposed and designed using hardware in loop simulation technique (Xia et al., 2003). Wu (2005) designed a multi-function process and control experiment system which is used for education and research.

At the same time, internet technology is used in simulation (Wang, 2007). Virtual real technology also has been used in chemical simulation (Liu, 2003).

These simulation systems above are used for operator training, chemical parameter optimization, implement of control strategy. However, how to evaluate the result becomes a problem. Some scoring algorithms and systems are proposed and developed (Li et al., 1999; Yu et al., 2007). These systems focus on different aspects of chemical process. The scoring knowledge are organized and stored in different ways. It is difficult to share and reuse the knowledge.

Ontology is a concept of philosophy. In philosophy, ontology is mainly concerned with existence itself. Owing to its ability to describe the basic concepts and relationship of a system, it has been applied in several fields such as information system et al. to fulfill the sharing and reuse of knowledge.

In the study, a novel general ontology-based automatic scoring framework is proposed. Scoring ontology is built according to scoring aspects (operation, control loop, safety, production and consumption). The knowledge can be shared and reused. The case study
shows that the framework can evaluate the results of operator training, chemical parameter optimization and implement of control strategy objectively and comprehensively.

**Ontology**

Ontology is the explanation of an existing system from a view of philosophy. Gruber (1993) proposed a widely used definition of ontology. It is a specification of a representational vocabulary for a shared domain of discourse. And then, Borst (1997) gave another definition: A formal specification of a shared conceptual model. Perez and Benjamins (1999) summarized five modeling primitives: Concepts, relations, functions, axioms, instances. There are four basic relations: Part-of, kind-of, instance-of and attribute-of.

Gruber (1995) has proposed the following specific rules that ontology should follow:

- **Clarity**: Using a natural language to define the intended meaning of ontological terms accurately, objectively, necessarily and sufficiently
- **Coherence**: The ontology model should be logically consistent and be able to sanction inferences that do not contradict the definitions
- **Expandability**: One should be able to define new terms for special uses based on the existing vocabulary without changing any existing definitions
- **Minimal encoding bias**: The conceptualization should be specified at the knowledge level without depending on a particular symbol-level encoding, so that it can be implemented in different representation systems and styles of representation while minimizing encoding bias
- **Minimal ontological commitment**: Ontology should require the minimal ontological commitment sufficient to support the intended knowledge-sharing activities

Owing to the ability of sharing and reuse of knowledge, the ontology technique has been applied in many areas, such as information organization, information research. In recent years, ontology has been used in chemical industry (Kitamura and Mizoguchi, 1999; Kuraoka and Batres, 2003).

**Ontology-based Automatic Scoring Framework**

In the section, an ontology-based automatic scoring framework is introduced.

---

**Scoring aspects**: The structure of a modern chemical plant is shown in Fig. 1
- **It includes**: Management, control system, SIS (safety instrument system), operation, communication network, measurement/actuating equipments and production equipments

Most of simulation systems are simulating the running of a real plant and used for operator training, chemical parameter optimization, implement of control strategy. In order to evaluate the result objectively and comprehensively, five basic scoring aspects are summarized according to the structure of a plant.

**Operation**: Operation is a very important issue for operator training. Operation needs to be evaluated during start-up process, stop process, fault maintenance.

**Control loop**: This aspect is used to evaluate performance of control loops.

**Safety**: Safety is an important issue for chemical simulation process. It evaluates whether some important variables have been in dangerous state.

**Production**: Production is used to evaluate the final production of the chemical simulation system.

**Consumption**: Consumption is used to evaluate the usage of raw material and energy.

**Scoring ontology**: Basing on the scoring aspects in the previous section, the scoring ontology is shown in Fig. 2.
Fig. 2: Scoring ontology

The five aspects are analyzed in detail to find the basic attributes and relations which is used for establishing the scoring ontology.

As it shown in Fig. 2, there are five basic concepts: Operation, control loop, safety, production, consumption. Every operation includes four attributes: Sequence condition, chemical condition, action and target. Sequence condition represents that the operation must be executed according to the sequence. Chemical condition means that operation can be executed until the chemical condition is satisfied. Action is to execute an operation. Target is used to describe the target of the operation. An operation can be finished until the action and target have been completed.

**Control loop includes:** Whether the controlled variable is steady and the curve after disturbance is added. When a disturbance is added, some parameters are calculated for evaluating the performance of control loops, such as decaying ratio, maximum deviation and so on.

**Safety includes four attributes:** high high limit, high limit, low low limit and low limit.

Fig. 3: Ontology-based scoring framework

The scoring ontology includes the basic scoring aspects for evaluation of operator training, chemical parameter optimization, performance of control strategy.

- **Scoring framework:** Basing on the scoring ontology, a framework is designed and shown in Fig. 3

As it shown in Fig. 3, scoring ontology is used to store the scoring knowledge. The input scoring knowledge is translated by knowledge acquire module.
Scoring inference engine is used for real time inference to evaluate the result of operator training, chemical parameter optimization and performance of control strategy.

**CASE STUDY**

In this part, the scoring framework is used to score for the furnace process.

The furnace process is a unit of SMPT-1000 (senior multi-function process and control training system). Its process is shown in Fig. 4.

The main chemical process is: the material A is sent through furnace and heated. Air and oil is sent into furnace and burn to supply heat. The flue gas is emitted through the chimney.

The heated product is used for other process. The process is controlled by a real DCS (distribute control system).

Take start-up process for example. The furnace simulation process is started and the scoring framework starts to work. The control loops are designed in DCS (automatic start-up program is not used when it is used for operator training). When the start-up process ends, the scoring result is shown in Table 1.

**Table 1: Scoring result**

<table>
<thead>
<tr>
<th>Operation</th>
<th>index</th>
<th>Sequence</th>
<th>Chemical condition</th>
<th>Action</th>
<th>Target</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>5</td>
</tr>
<tr>
<td>2</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>5</td>
</tr>
<tr>
<td>3</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>5</td>
</tr>
<tr>
<td>4</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>Finished</td>
<td>5</td>
</tr>
</tbody>
</table>

**Control loops**

<table>
<thead>
<tr>
<th>Variable</th>
<th>Recovery time</th>
<th>Maximum deviation</th>
<th>Decaying ratio</th>
<th>Steady</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>T1104</td>
<td>100</td>
<td>4.5</td>
<td>2.3</td>
<td>Yes</td>
<td>18.5</td>
</tr>
<tr>
<td>E1105</td>
<td>90</td>
<td>2.0</td>
<td>3.0</td>
<td>Yes</td>
<td>15.0</td>
</tr>
</tbody>
</table>

**Safety variable**

- High limit
- Low limit
- Beyond the limits

<table>
<thead>
<tr>
<th>Variable</th>
<th>High limit</th>
<th>Low limit</th>
<th>Beyond the limits</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>A1101</td>
<td>3%</td>
<td>1%</td>
<td>yes</td>
<td>0</td>
</tr>
<tr>
<td>P1102</td>
<td>600</td>
<td>10</td>
<td>yes</td>
<td>0</td>
</tr>
</tbody>
</table>

**Consumption**

<table>
<thead>
<tr>
<th>Variable</th>
<th>High limit</th>
<th>Low limit</th>
<th>Consumption</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1202</td>
<td>1500</td>
<td>900</td>
<td>1480</td>
<td>6.8</td>
</tr>
</tbody>
</table>

**Production**

<table>
<thead>
<tr>
<th>Variable</th>
<th>High limit</th>
<th>Low limit</th>
<th>Production</th>
<th>Score</th>
</tr>
</thead>
<tbody>
<tr>
<td>F1105</td>
<td>360000</td>
<td>180000</td>
<td>25000</td>
<td>9</td>
</tr>
<tr>
<td>No.</td>
<td>12345</td>
<td>total</td>
<td>69.3</td>
<td></td>
</tr>
</tbody>
</table>

---

Fig. 4: Furnace process
As it shown in Table 1, operation, control loops, safety, consumption and production are evaluated by the system. The scores of control loops are calculated according to recovery time, maximum deviation, decaying ratio.

CONCLUSION

Chemical simulation systems have been widely in operator training, chemical parameter optimization and implement of control strategy. In order to evaluate the result of operator training, chemical parameter optimization and performance of control strategy, an ontology-based automatic scoring framework is proposed.

A scoring ontology is built to ensure sharing and reuse of knowledge. It includes five basic concepts: operation, control loop, safety, production and consumption. Basing on the ontology, the scoring framework is designed. The case study shows that it can be used for automatic scoring in chemical simulation systems.

REFERENCES


