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A Framework for Agent-based Chemical Process Modeling

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Abstract: As the most chemical processes that we need to analyze and models are becoming more complex in terms of their interdependencies, conventional modeling methods may not be as applicable as they once were. Agent is now being considered as the most effective tool to design and build complex and distributed system. Agent-based architecture provides additional robustness, scalability, flexibility and is particularly appropriate for problems with a dynamic, uncertain and distributed nature. In this paper, a framework of agent-based modeling for chemical process is illustrated. The chemical process characteristics are classified systematically. The modeling elements, as well as semantics and graphical representations for each element are defined and described. And two cases in different scenarios of chemical process industry, including tank-level system and rectification system, are presented in the following section. Finally, several future research directions toward the successful deployment of agent technology in chemical process industry are discussed.

Key words: Chemical process, agent-based modeling, tank-level system, rectification column

INTRODUCTION

Nowadays, chemical processes are becoming more and more complex, due to the widely used sophisticated devices and control systems, to meet the ever-increasing demand for economic benefits. As the consequence of these changes, traditional modeling methods, such as knowledge based method, neural network, etc., are no longer effective as it is before. Agent, however, is now being considered as the most effective tool to design and build complex and distributed system (Macal and North, 2010).

Agent is an autonomous system suited in the specific environment and it is capable to meet its design objectives (Bonabeau, 2002; Wooldridge and Jennings, 1995). Although there are many definitions depicted by different researchers in various studies, most of them are in broad agreement (Wooldridge and Jennings, 1995; Jennings, 2000; Chen and Cheng, 2010). The agent has capability to acquire information from its environment, makes decision and response in a timely fashion to changes that occur in it. Agents collaborate with each other, sharing information, knowledge and tasks among themselves, to achieve common goals. Agent-based models consist of dynamically interacting agents. The systems within which they interact can create real world-like complexity. These agents are intelligent, purposeful and situated in space and time. They reside in networks and in lattice-like neighborhoods. The location of the agents and their responsive and purposeful behavior are encoded in algorithmic form in computer programs. Agent-based architecture provides additional robustness, scalability, flexibility and is particularly appropriate for solving problems with a dynamic, uncertain and distributed nature.

The agent-based modeling has been addressed in various engineering domains. Plenty of intelligent agent systems have been applied to many aspects of traffic and transportation systems, including modeling and simulation, dynamic routing and congestion management and intelligent traffic control (Shen *et al*., 2006). Agent-based collaborative configuration can also be widely applied in manufacturing automation, supply chain management and monitoring workflow (Tian and Tianfield, 2006; Wang *et al*., 2005), etc. In general, agent-based system is applicable more effectively in the case that there exist many design alternatives because decisions and conflicts caused by constraint violation should be tracked for management of design history.

Compared with other engineering domains, there has been little work and applications in process engineering. Most of these modeling activities and research focus on a narrow scope with little to no macro-level environment interaction and offer no guidance on how others can integrate agent-based modeling into their own research (Gabbar *et al*., 2003; Gao *et al*., 2005; Pogson *et al*., 2006). The remainder of this paper is structured as follows. First, we present the detailed description of our agent-oriented

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modeling methodology and the process of multi-agent system design, in section 2. Then in section 3, we focus upon the models that we have developed in two cases, one is tank-level system and the other is rectification system which are presented to show how to apply this method into actual chemical process. Section 4 discusses the future research activities of agent-based modeling in chemical process.

PROPOSED AGENT-BASED MODELING FRAMEWORK

Chemical process is a complex system which commonly has large vessels or sections called units that are interconnected by piping or other material-moving equipment which can carry streams of material. The output product is converted by raw material through a certain process. In this system, material flow, energy flow and information flow are transferred among these devices; thereby form a complex interaction network. The typical chemical process is shown below.

In Fig. 1, the blue lines represent the material flow while red lines represent the energy flow. Equipment and pipelines are the container and carrier of material, respectively. As for control system, they always have some intelligence and the information flow is transferred by them. After the highly abstract, the chemical process can decompose into equipment, material and control system. And thus, it offers a systematic basis for agent-based modeling.

MODEL ELEMENTS

Equipment: Devices act as the vital important role of the chemical process. They are connected by pipelines and realize the specific functions of the process. For example, the furnace is a device used to provide heat for a process or can serve as reactor which provides heats of reaction. The furnace itself includes some attributes, such as temperature, pressure, etc. and the heat reaction is the

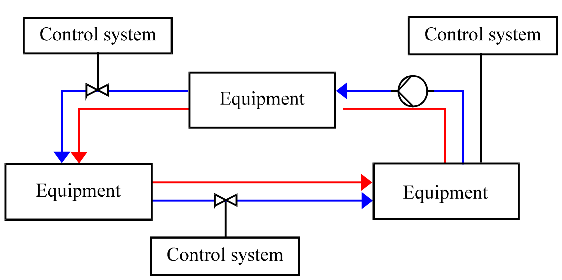

Fig. 1: Typical schematic diagram of chemical process

interaction activity taken place in the furnace. Every device has the characters of autonomous, responsive, social and proactive; such characters are consistent with the definition of the agent. So we view the equipment as the backbone of the agent-based model.

The equipment model is usually composed of attributes, behaviors and relations. It completes its functions and communicates with other related equipment, material, control system or environment. Different equipment has different attributes and result in different behaviors that it has.

Control system: A control system is a device or set of devices to manage, command, direct or regulate the behavior of other devices or systems. It monitors and affects the operational conditions of a given dynamical system. Here the control system agent can be viewed as the abstraction of the real system which generally comprises a series of devices, such as sensor, actuator, etc.

A control system will mainly have associated with some properties in control theory. For instance, if it contains PID controller, the proportional, integral, derivative parameters are the basic properties. The system obtains the desire output through the manipulations of controller.

From modeling perspective, control system can be considered as a perfect agent prototype. The control system has set point which can be taken as target of the agent; and control system operates the actuator to realize the objective. In the course of this realization, manipulations are seen as behavior of the agent. For example, a boiler control system might have a temperature setpoint which is the system aims to attain. The control system may trigger a series of mechanical actuators in the correct sequence to perform this task.

Material: The complex equipment usually contains more information. However, the model which is made up of equipment is still isolate and immethodical. Former modeling methods are accustomed to analysis devices in the process and take them for the subject of the model but ignore the effect of the material. This may often lead to the conflict of roles overlap that the devices are imposed with the some attributes which are not belonged to them. Therefore, we take the material into account for agent-based modeling.

Generally, material agent is to decouple the redundant material information from the equipment, so as to make the agent to be self-contained, modular and uniquely identifiable individual.

Environment: Agents interact with other agents and with their environment. The environment can simply be described as a simple container based on a set of semantic. From a modeling perspective, the environment represents an abstract population but they provide more richness. The agents in an environment are the population of a model.

Environment is hierarchical that it includes other sub-environment which is corresponding with the sub-system in the chemical process. Each of the sub-environments can have its own state that is separate from the state of its parent. The hierarchical means that a model component that is present in an environment is also present in that environment's entire parent environment. Of course, the converse is not true in the general case. The hierarchical structure itself can be declaratively or imperatively specified by the modeler. Environment membership and structure is completely dynamic and agents can be in any number of combinations of environment at any time.

In addition to supporting hierarchical nesting, environment can have behaviors associated with it. Generally, these behaviors would affect the internal state of the environment. For example, the environment that represents a furnace might have a burner model associated with it. This model would represent the behavior of the environment. The burner model would be driven by using the state of the environment and the output would update the state of environment. One could apply more complex or adaptive behaviors to an environment, thus giving the environment an agent-like quality. This provides a rather powerful mode of composition.

Environment also supports data layers. Data layers represent numerical data that can be accessed using a set of coordinates. Data layers allow model designers to provide numerical values with which their agents can interact. The data layers for a given environment are separate from the layers for other environment, allowing the agents to orient themselves with respect to a set of data depending on which environment they are using.

Relationship: Since, the agents within an environment likely interact across multiple sets of relationships, we deliberately designed them to not impose a particular structure on how the agents interact. The relationship is a data structure designed to define and enforce connection between agents within a given environment, whether it be spatial, network, or something else. In other words, an agent is realized once a relationship is applied to it. From a practical perspective, this means that relationship is added to an environment to allow the agents to interact with one another.

The relationship has a many-to-one connection with the environment. Each environment can have an arbitrary number of relationships associated with it which means that within each environment, the agent can create an arbitrary number of types of relationships with each other. However, an agent must exist in an environment before it can be used in a relationship. So, if an agent tries to work in a relationship before it has been added to the environment, it will fail. For example, if there has been a network and the model designer try to create a link between agents where at least one of the agents does not yet exist in the environment, then it will fail.

This model consists of a set of protocol definitions. That is, a pattern of interaction that has been formally defined and abstracted away from any particular sequence of execution steps. Viewing interactions in this way means that attention is focused on the essential nature and purpose of the interaction, rather than on the precise ordering of particular message exchanges.

MODELING ARCHITECTURE

Figure 2 presents the agent-based modeling architecture of chemical process. The modeling procedure can be divided into two stages, the analysis phase and the design phase. In the analysis phase, we convert the raw information into the classified information which are called equipment model, control system model and material model. However, these models are just the collection of information and more abstraction will be done in the design phase. That is, based on those intermediate states, we design the agent model and relationship model finally.

Analysis phase: The goal of this analysis stage is to gather and analyze the information of the process. In other words, in this stage, we classify the massive raw process information for modeling use. The desired outcoming is to set up the equipment model, material model and control system model. Here, we give a recommended analysis procedure as a template:

- **Divide the system:** Firstly, divide the system into several independent parts, or sub systems. The P and ID is a useful reference upon which a complex system can be divided into many structure and function

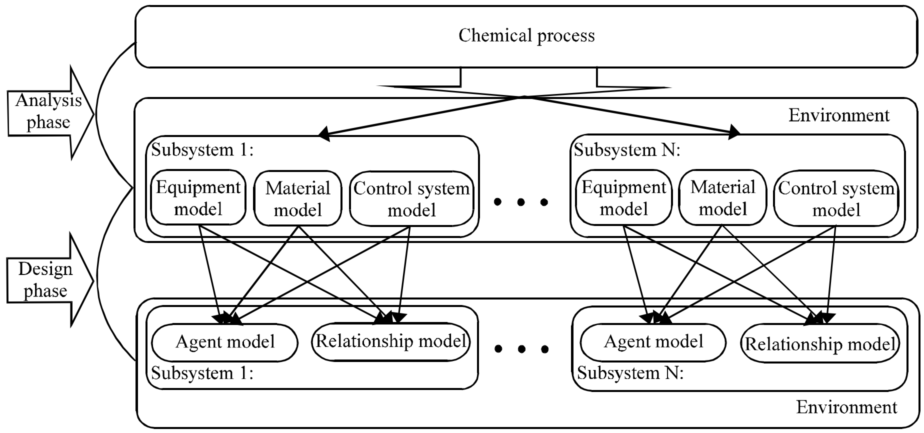

Fig. 2: Modeling architecture for chemical process

relative simple parts. The division is important because a good partition allow model engineers to focus their work on local systems

- **Classify the type of the element:** For each divided part, pick up the material, the devices and the control system which are analyzed one by one according to the flow of material carefully. Since, most of the subsystems realize the system functions through the core equipment, we take it for granted that all of the equipment should be selected as candidates. Moreover, some subordinate equipment also is possible to be selected which requires specific analysis
- **Complete the models:** After analysis the whole process, the models, equipment model, material model and control system model, are finished at the same time. Usually, we have some modification when the original model is done, so as to make it better expression

Design phase: Compared with the analysis phase, this stage is more important. The intermediate model which is expressed as equipment model, material model or control system model, will be finally abstracted and converted to agent-based model which include agent model and relationship model.

In an agent model, everything associated with an agent is either an agent attribute or an agent behavior that realize specific function. Agent attributes can be static, not changeable during the simulation, or dynamic, changeable as the simulation progresses. For instance, the agent's name is typically a static attribute; a dynamic attribute is an agent's memory of past interactions. The types of gent behaviors are various, such as rules or serials of actions. An example of the behavior is that a material agent acquires its location now.

In a relationship model, it concerns with modeling relationships and interactions between agents and also between agent and the environment. The two primary issues of modeling agent relationship is specifying connections between the agents and the mechanisms of the dynamics of the interactions. Agents interact with other agents but not all agents interact directly with all the other agents all the time, just as in real-world systems.

The environment may simply be used to provide public resources and information that agents will use when they are interacting. It also stipulates the constraints of the whole model. In our model structure, some equipment which is not as autonomy as a real agent, can be considered as a part of the environment.

At the end of the modeling procedure described above, we have to join up all the models of subsystems together, forming an integrated process model. In addition, the conflicts of the expression in the model are verified.

CASE STUDY

Here, we present a rectification case to describe proposed modeling process.

As shown in Fig. 3, rectification system is widely used in the chemical process industries where large quantities of liquids have to be distilled. Feed stream is separated into one distillate fraction and one bottoms fraction. The "lightest" products with the lowest boiling points exit from the top of the column and the "heaviest"

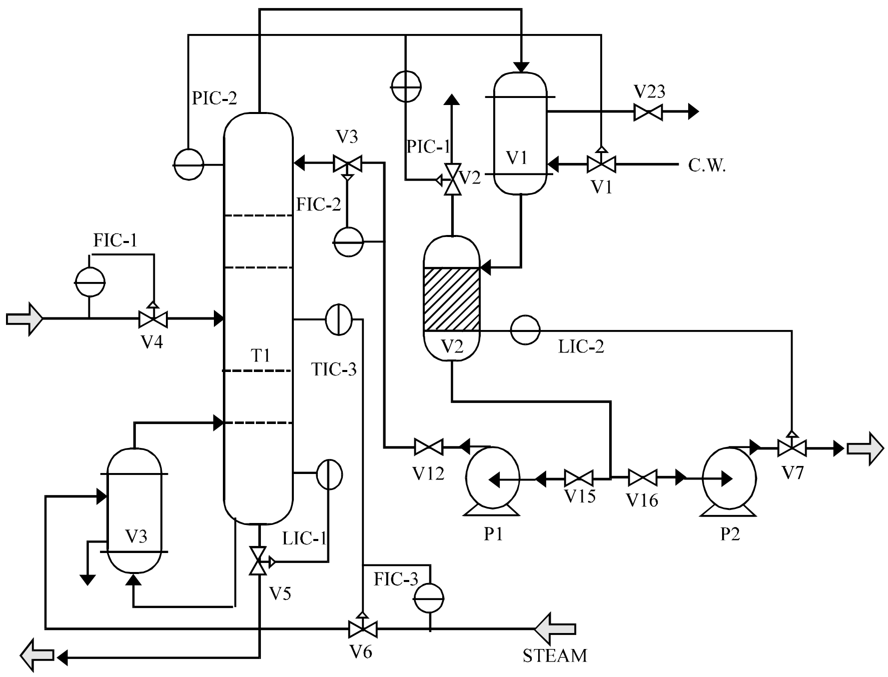

Fig. 3: Rectification system flow diagram

products with the highest boiling points exit from the bottom. Condenser is used to condense the distillate fraction from gaseous to liquid state, typically by cooling it. External reflux is used to achieve better separation of products. Reboiler is heat exchangers typically used to provide heat to the bottom of industrial distillation column. They boil the liquid from the bottom of a distillation column to generate vapors which are returned to the column to drive the distillation separation. The key variables of rectification system are listed as Table 1.

This is a relatively complex system. In this process, there are three kinds of control system, including single loop control, cascade control and override control. As of equipment, they are distillation column, reflux tank, condenser and reboiler. The materials exist in this system are mixtures of hydrocarbons which are mainly C4, C5, C6 and C7. The distillate fraction is mainly C4 while the bottoms fraction is the others. Besides, cool water and steam in this system are used for heat exchange.

The agent model is shown in Fig. 4. This process is divided into four subsystems. All of the subsystems are centered with the critical devices in this process; they are distillation column, reboiler, condenser and reflux tank, respectively. As is illustrated previously, the one-way arrow represents the material flow direction in the system and the two-way arrow means the interaction between the two agents it links.

Table 1: Key variables of rectification system

Symbol	Definition
T1	Distillation column
V1	Condenser
V2	Reflux tank
V3	Reboiler
P1	Reflux pump
P2	Produced product pump
LIC-1	Level controller of distillation column bottom
LIC-2	Level controller of reflux tank
PIC-1	Pressure controller of distillation column (high)
PIC-2	Pressure controller of distillation column (normal)
FIC-1	Flow controller of feed
FIC-2	Flow controller of reflux
FIC-3	Steam flow controller of reboiler
TIC-3	Temperature controller of distillation column

According to the types of agent defined in the previous part, we can obtain cool water agent, steam agent and feed agent which are instances of material agent; equipment agents are distillation column agent, condenser agent, reboiler agent, etc. And there are also some control system agents, such as FIC-1 agent, PIC-1 agent, LIC-1 agent, etc. Each agent in the model is derived from the corresponding template that we have set and then have some modification on that basis, thus, it is unnecessary to give more details here.

From the agent model, we can find that there are a number of interactions between agents. All of these are detailed in the relationship model. For example, the interaction between FIC-3 agent and steam agent is shown in Fig. 5, a sample of the relationship model.

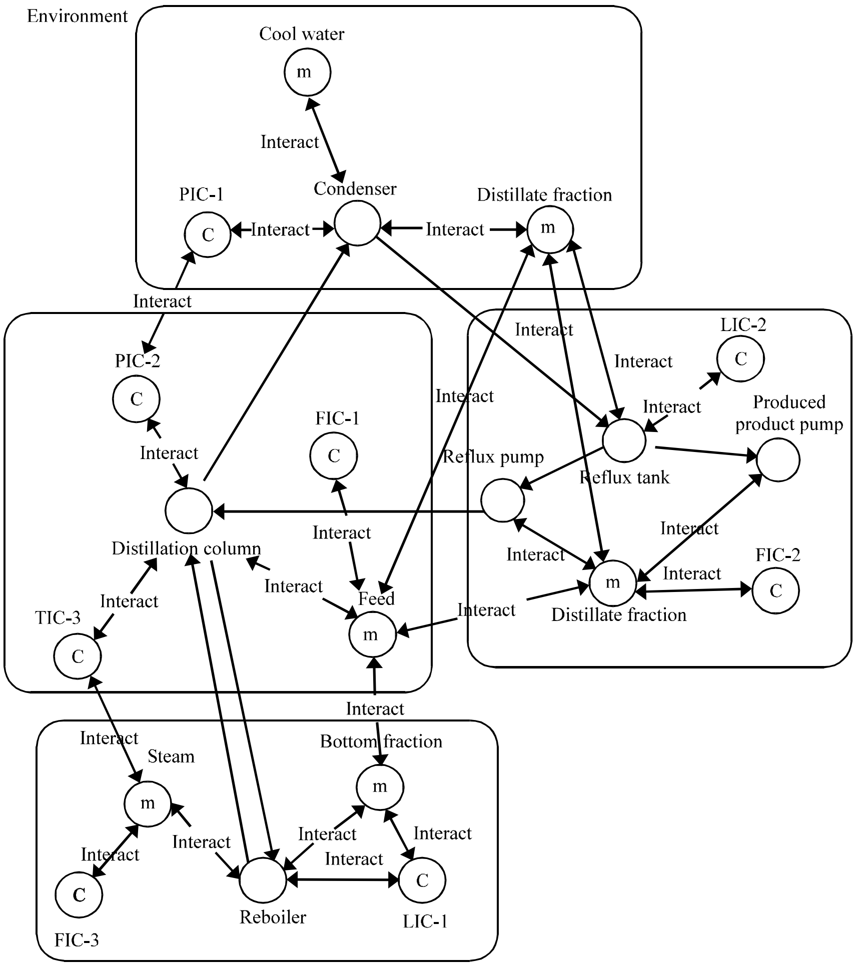

Fig. 4: Agent-based model of rectification system

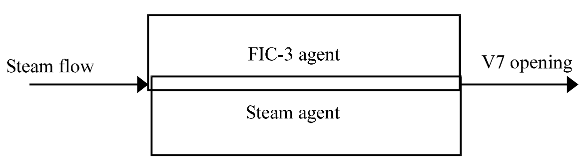

Fig. 5: Relationship model in rectification system

This states that the interaction is initiated by FIC-3 agent and involves steam agent. Steam flow and Valve V7 opening are the input and output of the interaction, respectively.

CONCLUSION AND FUTURE WORK

In this study, we have described a modeling framework that allows the analyst to capture chemical process characteristics effectively. For this, we classified chemical process characteristics systematically. We defined modeling elements such as equipment, material, control system, environment and relationship between agents and described semantics and graphical representations for each modeling element. To demonstrate how our modeling framework can be applied to a real case, we carried out a case study over real chemical processes.

Although, this study may have some limitations, the proposed framework for the chemical process can serve as a useful modeling tool that overcomes the limitations of traditional modeling techniques. As further research, the following can be considered. First, more detailed characteristics of the chemical process and relevant modeling elements and parameters can be developed. Second, an efficient automatic model verification method is necessary.

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