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Vinyl Acetate Monomer (VAM) Plant Model: A New Benchmark Problem for Control and Operation Study

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Abstract: A rigorous dynamic plant model of a vinyl acetate monomer (VAM) production was developed. This plant model enables the users to experience realistic plant operation, since it reflects the real plant characteristics and practical problems on the basis of experienced practitioners' opinions. More importantly, the plant model provides a new benchmark problem; the users can investigate start-up/shut-down operation, plant-wide process control, fault detection and diagnosis, and others. Multiple scenarios prepared in the developed model cannot be simulated in conventional benchmark problems. The plant model can be used also for chemical engineering education. This advantageous plant model is released from Omega Simulation Co., Ltd. with a free limited license of Visual Modeler, which is a commercial dynamic simulator and can be linked with MATLAB®. This article aims to introduce the VAM plant model, the steady-state balance, various disturbances and malfunctions, and operation scenarios.

Keywords: Process simulators, process models, dynamic models, benchmark examples, chemical industry, plant-wide control.

1. INTRODUCTION

A test problem which checks the industrial relevance of new ideas and technical developments is of great importance in the study of process control and process data analysis. A great number of researchers have utilized the Tennessee Eastman challenge problem in various fields including plant-wide control, production efficiency optimization, soft-sensor design, fault detection and diagnosis, etc., since it was introduced more than 20 years ago (Downs and Vogel, 1993). Even now, the Tennessee Eastman problem is the most popular problem. Later, Luyben and Tyreus (1998) developed a model of a vinyl acetate monomer (VAM) plant, which is a larger system containing standard chemical unit operations for real chemical components. The process design background is well-established in the original paper. Several studies on control system design for this plant have been conducted (Chen and McAvoy, 2003; Olsen *et al*., 2005; Seki *et al*., 2010; Tu *et al*., 2013; Psaltis *et al*., 2014).

This paper introduces the advanced VAM plant model, which is implemented on the commercial dynamic simulator, Visual Modeler (Omega Simulation Co., Ltd.), as a new benchmark problem in lieu of the Tennessee Eastman problem. Visual Modeler has found many applications in industry as an operator training simulator. It is capable of handling various modes of plant operations including start-up/shut-down as a prerequisite of the operator training system, whereas the simulator attempts to keep the fidelity of the rigorous nonlinear model as high as possible. The dynamic simulator makes a good compromise between the model accuracy and solvability. We improved the VAM plant model developed by Yumoto *et al.* (2010) with reference to practitioners' opinions to make realistic operation scenarios. The new VAM plant model has the following features, which the Tennessee Eastman process model cannot cope with:

- It can simulate transient operations including start-up and shut-down.
- It can generate noises and disturbances with such realistic sources as measurement noise of sensors, non-ideality in actuators such as valve dead band, daily temperature fluctuations, etc.
- It can simulate various failure modes, which are set on the basis of the advice of experienced engineers and plant operating personnel.
- It provides an operator interface, which mimics a control room of real plants, so that the users can experience "real" plant operations.

In the next section, the VAM plant is described. In section 3, details of the dynamic model implemented on Visual Modeler are explained, including static balance and process flow diagram. Section 4 shows operation scenarios and also demonstrates an example of start-up operation. In section 5, summary of supporting environment for the users is described. Finally conclusions are drawn.

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2. VAM PLANT

Figure 1 shows the overall process flow diagram of the VAM plant, which firstly generates VAM product in the reactor, then separates the product from the unreacted materials and by-products by using the distillation column and other units.

2.1 Process Overview

Eight materials appear in the VAM plant as shown in Table 1. Three raw materials are introduced to the process. Ethylene (C2H4) and oxygen (O2) are fed in the gas phase; acetic acid (AcOH) is fed in the liquid phase and vaporized with superheated steam at the vaporizer. These three materials are mixed and introduced to the reactor, in which the following gas phase reactions are taking place.

[Main reaction]
$C_2H_4 + CH_3COOH + 1/2O_2$
$\rightarrow CH_2{=}CHOCOCH_3 + H_2O$
[Side reaction]
$C_2H_4 + 3\ O_2$
$\rightarrow 2CO_2 + 2\ H_2O$

The main reaction generates VAM (CH2=CHOCOCH3) product and by-product water (H2O) from C2H4, AcOH (CH3COOH), and O2. The side reaction generates by-product carbon dioxide (CO2) and H2O from C2H4 and O2. Both reactions are exothermic, thus reaction heat is removed by boiler feed water (BFW) circulation and steam is generated at the shell side of the reactor. The reactor outlet gas containing about 5mol% VAM product is cooled down to 37degC with two coolers. Unreacted AcOH, H2O, and VAM are condensed as liquid VAM crude at the separator. On the other hand, separated gas leaving from the separator includes unreacted C2H4, O2, by-product CO2, inert ethane (C2H6), and a small amount of uncondensed VAM. This separated gas is compressed by the compressor to circulate recycle gas flow, then introduced to the absorber. The uncondensed VAM is absorbed by the cold AcOH which is fed from the top of the absorber. The mixture of VAM and AcOH is discharged from the bottom of the absorber, and mixed with the VAM crude at the intermediate buffer tank.

Table 1. Materials in the VAM plant

Material	Description
Ethylene (C2H4)	Raw material of VAM
Oxygen (O2)	Raw material of VAM
Acetic Acid (AcOH)	Raw material of VAM
VAM	Product
Water (H2O)	By-product
Carbon Dioxide (CO2)	By-product
Ethane (C2H6)	Accompanying gas of Ethylene
Nitrogen (N2)	Inert gas

Part of VAM removed from the top of the absorber is recycled to the inlet of the process. The remaining part of gas is introduced to the CO2 remover and the gas purge system, which keeps concentration of CO2 around 5~10mol% and C2H6 around 5mol% in the gas recycle line. The VAM crude at the intermediate buffer tank is fed to the azeotropic distillation column. VAM-H2O mixture discharged from the top of the column is condensed at the condenser and separated at the decanter. VAM forms the organic phase and H2O goes to the aqueous phase; VAM product is discharged as organic product from the decanter. Unreacted AcOH is discharged from the bottom and recycled to both the vaporizer and the absorber.

2.2 Process constraints

The VAM process must be operated under the following constraints, which come from safety, equipment protection, and product quality requirements.

- The O2 concentration must not exceed 8mol% anywhere in the gas pipeline to avoid an explosion.
- Pressure in the gas pipeline must not exceed 862kPaG because of the mechanical construction limit.
- The peak reactor temperature must remain below 200degC to prevent damage to the catalyst.
- The reactor inlet temperature must remain above 130degC to avoid dew point of AcOH.
- The AcOH concentration in the VAM product must remain below 150ppm as a product specification.
- The VAM concentration in the bottom of the distillation column must remain below 100ppm to prevent polymerization of VAM.
- The compressor must run while O2 is remaining in the gas pipeline to avoid forming of O2 hot spot and explosion.

3. IMPLEMENTATION OF THE VAM PLANT MODEL

The VAM plant model was implemented with Visual Modeler (Omega Simulation Co., Ltd.), which is the commercial dynamic simulation software package, with reference to the process configuration and the static balance proposed by Luyben and Tyreus (1998). In addition, the VAM plant model was arranged with reference to actual issues and opinions from the fields of Japanese chemical industry to make the model and operation scenarios more realistic than the original as follows.

- Tuning the steady-state balance
- Adding pipelines and units for start-up operation
- Adding disturbances and malfunctions for abnormal situation operation