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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.

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

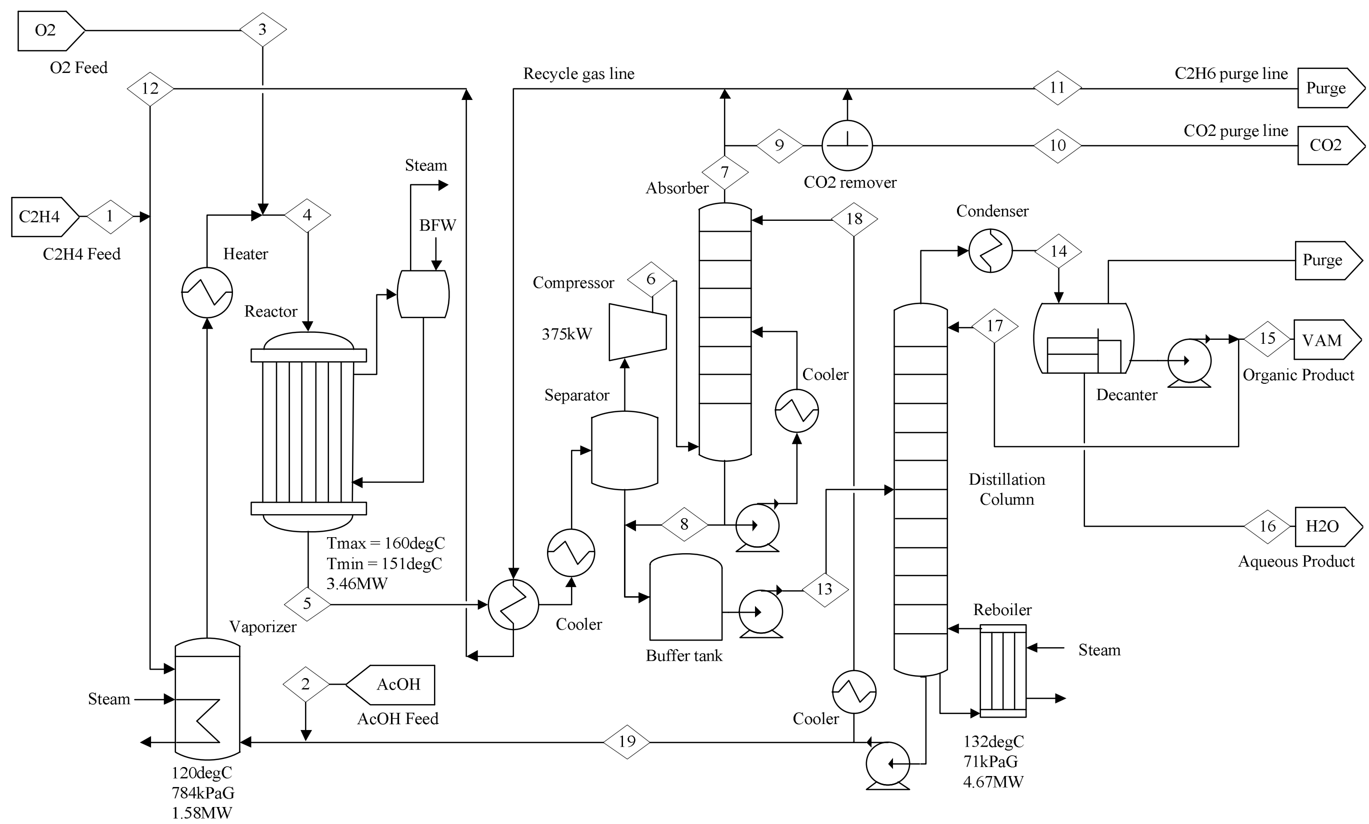

Fig. 1. Process flow diagram of the VAM plant

Table 2. Representative steady-state stream data. New balance / Original balance (Luyben and Tyreus, 1998)

		C2H4 feed	AcOH feed	O2 feed	Reactor inlet	Reactor outlet
Stream number		1	2	3	4	5
Flow	[kmol/h]	59.4 / 49.9	55.5 / 47.1	35.4 / 31.2	1143 / 1159	1116 / 1137
Temperature	[degC]	30.0 / 30.0	30.0 / 30.0	30.0 / 30.0	148.5 / 148.0	156.8 / 154.9
Pressure	[kPaG]	933.0 / 931.0	1299 / 931.0	933.0 / 931.0	783.1 / 783.1	525.5 / 518.2
O2	[mol%]	0.000 / 0.000	0.000 / 0.000	1.000 / 1.000	0.060 / 0.074	0.029 / 0.051
CO2	[mol%]	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.058 / 0.007	0.064 / 0.011
C2H4	[mol%]	0.999 / 0.999	0.000 / 0.000	0.000 / 0.000	0.709 / 0.584	0.674 / 0.553
C2H6	[mol%]	0.001 / 0.001	0.000 / 0.000	0.000 / 0.000	0.051 / 0.214	0.052 / 0.218
VAM	[mol%]	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.001 / 0.002	0.052 / 0.042
AcOH	[mol%]	0.000 / 0.000	1.000 / 1.000	0.000 / 0.000	0.114 / 0.110	0.066 / 0.072
H2O	[mol%]	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.007 / 0.009	0.062 / 0.053
N2	[mol%]	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000

		CO2 purge	C2H6 purge	Column feed	VAM product	H2O product
Stream number		10	11	13	15	16
Flow	[kmol/h]	4.78 / 5.10	0.93 / 0.18	240.7 / 229.2	58.5 / 49.6	58.7 / 49.9
Temperature	[degC]	38.0 / 40.0	38.0 / 40.0	39.3 / 42.5	41.0 / 40.0	41.0 / 40.0
Pressure	[kPaG]	815.4 / 781.3	815.4 / 781.3	59.1 / 477.8	22.7 / 22.8	22.7 / 22.8
O2	[mol%]	0.000 / 0.000	0.036 / 0.059	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000
CO2	[mol%]	1.000 / 1.000	0.072 / 68 ppm	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000
C2H4	[mol%]	0.000 / 0.000	0.821 / 0.667	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000
C2H6	[mol%]	0.000 / 0.000	0.064 / 0.266	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000
VAM	[mol%]	0.000 / 0.000	0.002 / 0.002	0.234 / 0.206	0.963 / 0.950	0.002 / 0.002
AcOH	[mol%]	0.000 / 0.000	0.004 / 0.005	0.466 / 0.513	23.0 ppm/370 ppm	16.1 ppm/370 ppm
H2O	[mol%]	0.000 / 0.000	0.001 / 0.001	0.300 / 0.281	0.037 / 0.050	0.998 / 0.998
N2	[mol%]	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000	0.000 / 0.000

Table 3. Modification of the steady-state balance

Changing points	Affected streams	Backgrounds
Reduce C2H6 concentration	4, 5, 6, 7, 9, 11, 12	C2H6 concentration is remained 2 to 5mol% in the actual process. In the past model, C2H6 concentration was more than 21% and it was decreasing efficiency of reaction. C2H6 concentration is remained around 5mol% in the new balance.
Increase CO2 concentration	4, 5, 6, 7, 9, 10, 12	CO2 concentration is remained around 5 to 10mol% in the actual process. In the past model, CO2 was removed perfectly with the CO2 remover, but it was not reasonable balance. CO2 concentration is remained around 6.0mol% in the new balance.
Increase C2H4 concentration; Decrease O2 concentration	1, 2, 3, 4, 5, 6, 7, 9, 10, 12, 13, 14, 15, 16, 17	VAM reaction efficiency is improved due to changing C2H6 and CO2 concentration as above. It enables to produce more VAM product with lower O2 feed concentration. As a result of modification, VAM production is increased 20% and raw material feed flow balance is changed. This improvement also affect to feed composition and operation condition of the distillation column.
Tighten specification of VAM product	15	AcOH concentration in VAM product is tightened from 600ppm to 150ppm by reference to actual product specification.

3.1 Tuning steady-state balance

Table 2 shows the steady-state material balance of both the new VAM plant model and the original balance proposed by Luyben and Tyreus (1998). Table 3 shows representative modifications of the steady-state, which is the important target profile for the start-up operation.

3.2 Adding pipelines and units for start-up operations

To make operation scenarios more realistic, the following pipelines and units are added to the plant model.

- [Configuration of the AcOH vaporizer]
  The AcOH vaporizer was expressed with two unit models, i.e., a heat exchange unit and a vapor-liquid separation unit, in the original model (Yumoto *et al*., 2010). In the new plant model, the vaporizer is expressed with a single unit model that can calculate heat exchange and separation simultaneously.

- [Start-up/shut-down lines]
  Several start-up/shut-down lines were implemented to realize realistic start-up/shut-down operation procedures. In the distillation column, for example, an initial product charge line and an emergency deliquoring line were added to the decanter vessel.

- [Intermediate buffer tank before the distillation column]
  An intermediate buffer tank is equipped between the reaction section and the separation section in many chemical processes to alleviate disturbances from the reaction section to the separation section. A new intermediate buffer tank was added before the distillation column as the same manner of the real process. This intermediate tank can be bypassed by switching lines around the vessel on demand.

3.3 Adding disturbances and malfunctions for abnormal situation operation

Tables 4 and 5 show disturbances and malfunctions, which were implemented on the new VAM plant model. The users can activate any single or multiple events at any time, not only during steady-state operation but also during start-up/shut-down operation. The users can flexibly change parameters of disturbances and malfunctions such as magnitude, time constant, and timing of recovering. The disturbances are coming from outside of the VAM process, such as changes in temperature and pressure of utilities. Thus, the control system should be designed to suppress these disturbances. On the other hand, process failure caused by malfunctions such as pump trip cannot be suppressed by control, so fault detection and diagnosis are needed. The users are able to investigate various issues related to process control, process monitoring, and others by using these malfunctions and disturbances.

4. OPERATION SCENARIOS

The VAM plant model can provide realistic operation scenarios, which cannot be investigated in conventional benchmark problems. The users can experience various real operation of the VAM plant as if they are operators of the real plant.

4.1 Initial state

The VAM plant model has initial state files which include information of all units and streams. The users need to load following initial state files before starting operation.

- [Before start-up]
  This initial state is prepared for start-up operation. All process units remain shut-down condition at this state.

- [Steady-state]
  This initial state is the steady-state described in Table 2.

Table 4. Disturbance list

No	Description	Pattern
1	Change C2H4 feed composition	Step/Ramp
2	Change AcOH feed composition	Step/Ramp
3	Change C2H4 feed pressure	Step/Ramp
4	Change O2 feed pressure	Step/Ramp
5	Heavy rain	Step/Ramp
6	Change cooling water temperature	Step/Ramp
7	Change cooling water feed pressure	Step/Ramp
8	Change 1.5MPa steam feed pressure	Step/Ramp
9	Change 5.0MPa steam feed pressure	Step/Ramp
10	Change 1.5MPa steam temperature	Step/Ramp
11	Change 5.0MPa steam temperature	Step/Ramp

Table 5. Malfunction list

No	Description	Pattern
1	Reduce reaction activity	Step/Ramp
2	Reduce heat transmission in vaporiser	Step/Ramp
3	Accident error of temperature sensors	Step/Ramp
4	Stop absorber circulation pump	Step
5	Stop column feed pump	Step
6	Stop column bottom pump	Step
7	Stop column reflux pump	Step
8	Stop compressor	Step
9	Stick separator bottom valve	Step
10	Stick absorber bottom valve	Step
11	Stop analysing sensors	Step
12	Failure of gas feed pressure sensor	Step
13	Failure of column reflux flow sensor	Step
14	Failure of column bottom level sensor	Step
15	Crack weir of decanter	Step
16	Increase differential pressure of column	Step/Ramp
17	Decrease efficiency of CO2 removal	Step/Ramp
18	Measurement error of column bottom level sensor	Step/Ramp
19	Measurement error of vaporiser level sensor	Step/Ramp

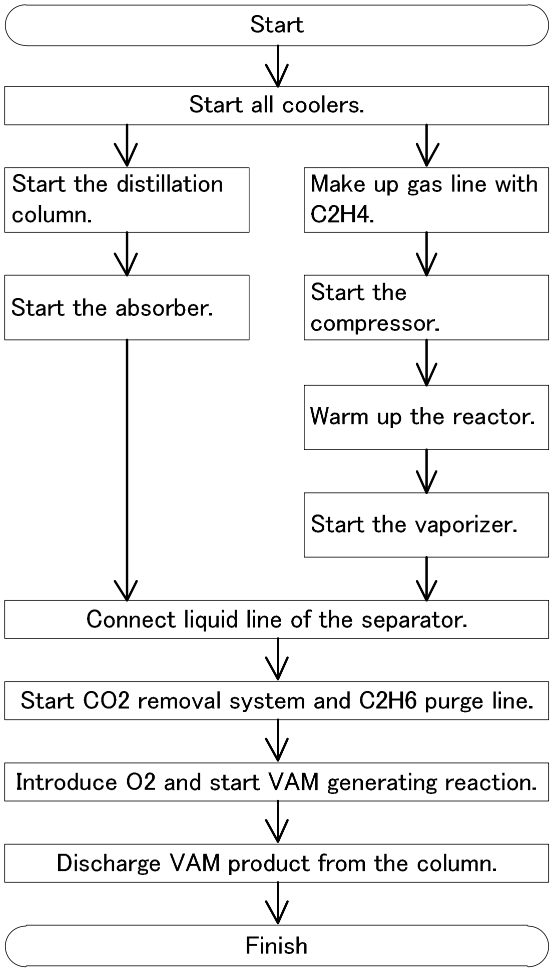

Fig. 2. Start-up operation procedure of the VAM plant

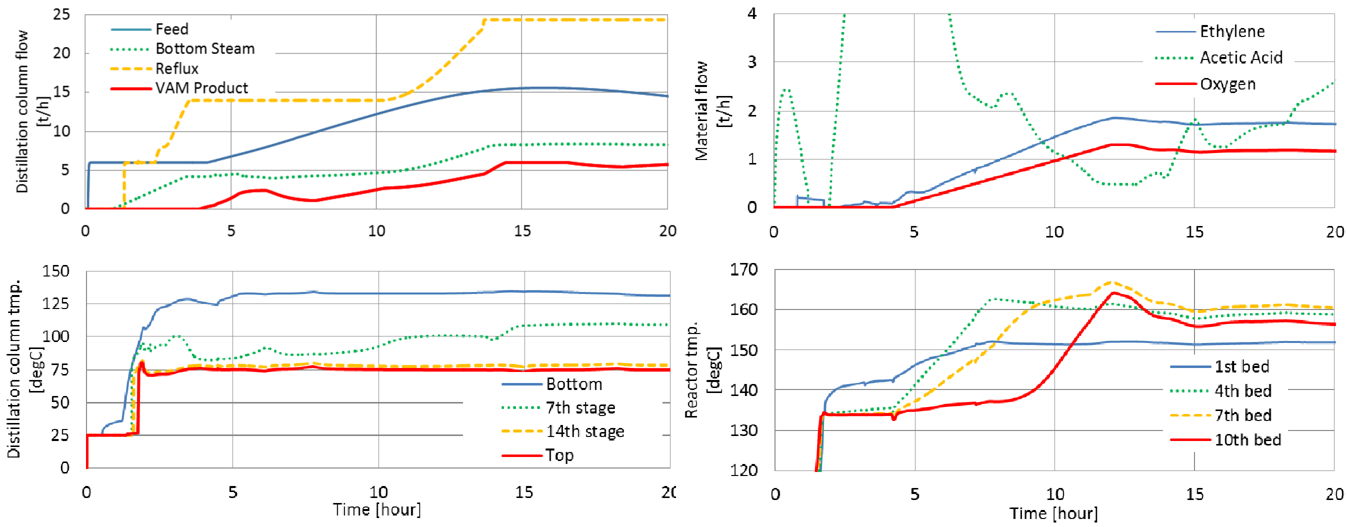

Fig. 3. Time-series data of start-up operation

4.2 Start-up operation

Figure 2 shows the outline of start-up operation procedure of the VAM plant model. Total time to finish this operation procedure is almost 20 hours, but the users can accelerate the speed of simulation calculations up to 200 fold in the case of time-consuming procedure, such as liquid filling of vessels and unit warming up. This operation procedure must be executed under process constraints described in section 2. Figure 3 shows representative time-series process data during the start-up operation.

4.3 Production load-up/load-down operation

The users can execute load-up/load-down operation from the steady-state. Production load of the VAM process can be increased by raising the O2 feed concentration and the reactor temperature. Load-down operation is totally opposite. After changing operation condition of the reactor, the distillation column condition should be adjusted in conformity to reactor load. This operation scenario will be a good example to investigate the plant-wide control loop configuration.

4.4 Abnormal situation operation

The users can start a simulation of the VAM plant model from the steady-state initial condition and experience abnormal situation operation by triggering disturbances and malfunctions at anytime. The users can study dynamic behavior caused by such disturbances and malfunctions, and also they can configure control logic and fault detection logic on the custom calculation blocks which are supported on the VAM plant model.

5. SUPPORTING ENVIRONMENT FOR THE USERS

The following elements are available on the Omega Simulation Co., web site for free.

- The VAM plant model with a free limited license of Visual Modeler.
- Time-series data sets for data analysis study including fault detection and diagnosis.
- Explanation documents to use the VAM plant model, which include process description, operation procedure, system manual, and so on.

We are also developing interface which links the VAM plant model and MATLAB®. This interface will be helpful to test control logics developed on MATLAB® as if it is applied to the real plant.

6. CONCLUSIONS

A rigorous plant model of vinyl acetate monomer (VAM) process was developed. The users can get feelings of the real plant operation through this model. It can also be used as a test environment for various studies in the process control field, such as plant-wide control, process monitoring, optimal operation, and so on. The developed VAM plant model with a free limited license of Visual Modeler is already available through the web site of Omega Simulation Co., Ltd.: http://www.omegasim.co.jp/contents_e/product/vm/cnt4/
(Official site : http://www.omegasim.co.jp/index_e.htm)

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