



## DYNAMIC SIMULATION OF DISTILLATION COLUMN UNIT TO STUDY OPERATIONAL FAILURES

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Distillation column units present special safety hazards because of their large inventories, which often involve flammable solvents. Thus study of operational failures, which may result into incidents or accidents, in a distillation column unit by simulation is of value. In such cases, a mandatory condition in safety assessment is the detailed disturbance analysis through simulation to cover a wide range of operation. In this paper, scenarios such as loss of cooling, more or less steam flow rate, high or low feed flow rate etc. are simulated to evaluate control structures and for safety examination. This is achieved through introduction of small and large disturbances. The distillation column unit, which is part of a hydrocarbon recovery plant, from a real chemical plant is taken for case study. The operational failures in distillation column unit under study were identified through simulation with two different inferential configurations and a dual composition control scheme. Simulation results illustrate that the condenser level controller, sump level controller, temperature controller and vent to atmosphere keeps the process controlled variables at the set point for these disturbances except for the case where 20% reduction in feed was introduced.

**Keywords:** Disturbance simulation, Safety analysis, Aspen dynamics, Loss of cooling medium, Over pressure

### 1. Introduction

Simulation is a basic activity in Process Engineering. In recent years, it is becoming an important tool for examining process operability, control alternatives and safety examination [1]. Figure 1 shows the different process simulation targets of simulation studies.

Three major integrated simulation systems widely used in the firms and companies for process simulation are Aspen technology (Aspen Plus, Aspen dynamics etc). Hysprotech (Hysys process, Hysys plant etc.) and Simulation Sciences (Pro/II etc.). Among these Aspen Dynamics is a powerful and easy to use tool, which enables users to realize the benefits of dynamic simulation. It is tightly integrated with Aspen Tech's steady state simulator Aspen Plus™. Within Aspen Plus™, steady state simulations can be casted into dynamic simulation in Aspen Dynamics by specifying additional engineering detailed parameters, including pressure/flow relationship, and equipment dimensions. Normally, dynamic process model developed in Aspen Dynamics is used for examining process operability, control alternatives and not used for trouble shooting of operational problems. Because of this, applications of simulation tool like Aspen Dynamics for analysis

of safety related process malfunctions might not describe reality. Thus, process disturbance simulation should be used for trouble shooting of operational problems and analysis of safety related process malfunctions. Process disturbance simulation means use of dynamic simulation to study physical effects of large variations e.g. flow with respect to maximum/ no flow and loss of cooling water instead of small disturbances for control loop tuning or control system design. Physical effects like under-pressure which results to reverse flow have to be considered in disturbance simulation but may be neglected for control loop tuning or in normal dynamic simulation. The analyst has to review the appropriate aspects of model and efforts must be made to validate the model in the area of application. Before using the dynamic simulation results in the safety analysis, the user should be aware of the underlying assumptions that are built into the dynamic simulation program code and how they affect the results. It may be necessary to perform several simulation runs and perform sensitivity analysis with respect to control responses in order to identify appropriate control response. In general, no credit is taken for automatic control action unless it tends to increase the risk. Several researchers [3-5] used dynamic

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simulation for safety analysis.

Distillation column units dominate in refineries and chemical plants and present special safety hazards because of their large inventories, which often involve flammable solvents. Thus study of operational failures, which may results into incidents or accidents, in a distillation column unit by simulation is of value. In this paper, a distillation column unit, which is part of a hydrocarbon recovery plant, from a real chemical plant is taken to illustrate the power of process simulation for design, control and safety analysis.

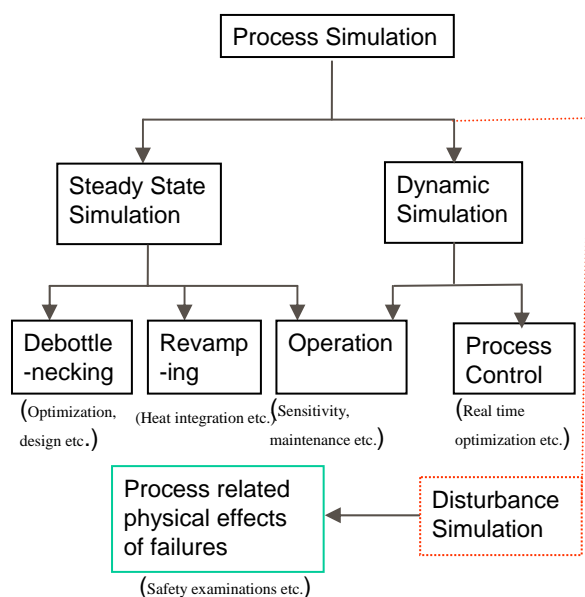


Figure 1. Applications of process simulation [2].

## 2. System Description

The unit under discussion is part of a hydrocarbon recovery plant, which removes hydrocarbons and other solvents from the off-gases of the distillate fraction plants (see Figure 2). Water, acetone, methanol, and acetic acid are the main components of the feed stream. The product stream (acetone rich) is separated from the effluent by using live steam injection. The column has a diameter of 0.728 m and consists of 35 trays. The live steam is entered at stage 35 (the stages are numbered from top to bottom) at a temperature of 141 °C and a pressure of 375 kPa. The feed, which is at its bubble point, is entered at stage 16 with a column head pressure of 100 kPa. The separation targets (mass %) are:

Distillate: Water < 10%

Base: Acetone < 2000 ppm

Methanol < 2%

Acidity < 3%

Where acidity is the sum of the mass fraction of the acids i.e. acetic acid, formic acid, and propionic acid in the base stream.

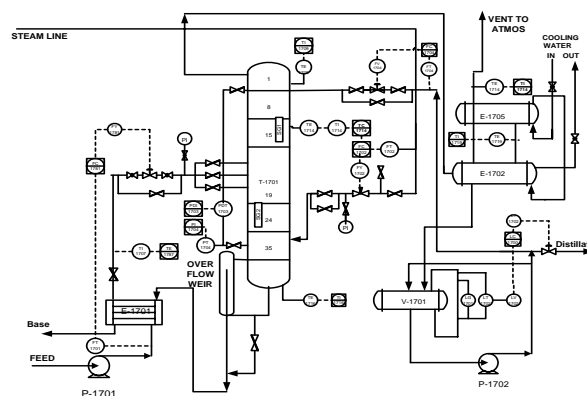


Figure 2. Process flow diagram of distillation unit.

## 3. Process Dynamic Simulation

First a tray by tray steady state process simulation model is developed using RADFRAC in AspenPlus™.

This steady state simulation model is used to find the optimum reflux ratio (0.7) and steam rate (589 kg/h) which strictly meet the specified separation targets of key components. Then additional information related to reflux drum, column sump and tray geometry is provided to cast the Aspen Plus™ steady state simulation model into dynamic simulation model. Figure 3 shows the Aspen Dynamics simulation model developed with somewhat modified control scheme. This dynamic model is first used for dynamic simulation of normal small disturbances to check the stability of control systems. Later on, it is used for disturbance simulation.

To evaluate the dynamic performance of the control structure, disturbances in feed flow rate and acetone composition in feed are imposed on the system. These disturbances are imposed on the system by removing feed flow rate controller and introducing step change in the variable of interest. At simulation time  $t = 1$  h, the following disturbances in feed stream are introduced and studied one by one:

- Step up change of 20 % in feed rate i.e. feed flow rate is increased from 4020 to 4824 kg/h.
- Step up change of 20 % in acetone composition in feed, keeping the feed flow rate constant and adjusting the other components composition so that the sum of all component concentration is one.
- Step down change of 20 % in feed rate i.e. feed flow rate is decreased from 4020 to 3216 kg/h.
- Step down change of 20 % in acetone composition in feed, keeping the feed flow rate constant and adjusting the other components composition so that the sum of all component concentration is one.

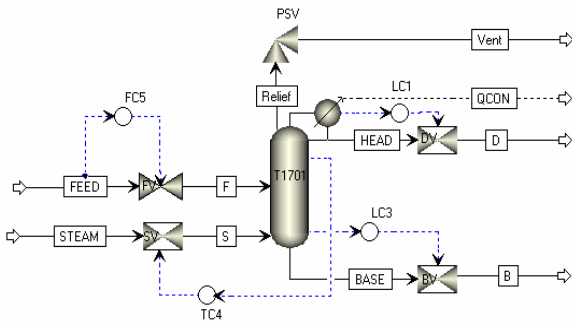


Figure 3. Aspen Dynamics Simulation Model.

The degree of effectiveness of control structure to handle these disturbances is analyzed from the dynamic response of controlled and manipulated variables along with key process variables. The dynamic simulation results illustrates that the condenser level controller, sump level controller, temperature controller and vent to atmosphere keeps the process controlled variables at the set point for all these disturbances except for step down change of 20% in feed rate. Thus dynamic response of the key process variables only for step down change of 20 % in feed rate is described here and simulation results of other disturbances is explained in somewhere else [6].

Figure 4(a-h) gives dynamic response of the key process variables for the disturbance of step down change of 20% in feed rate. When this disturbance is introduced into the system (see Figure 4(a)), the column head pressure reduces from atmospheric pressure to ~ 92 kPa (see figure 4(a)). As a result the downstream pressure becomes greater than the column head pressure so distillate flow falls down. This leads to flooding of condenser (see figure 4(c)) and condenser level

controller fails to kill this disturbance. Similar behavior is observed for sump level controller (see figure 4(e)), which leads to flooding at column base. The temperature controller works satisfactorily (see figure 4(g)). In the real plant, a pump is installed for the transfer of distillate and reflux so the problem of flooding of condenser will not occur. The flooding at column base will also not occur due to operation at ambient pressure (as in real plant) and by installation of bottom product pump. The dynamic response of system for less feed disturbance signifies the importance of pressure control.

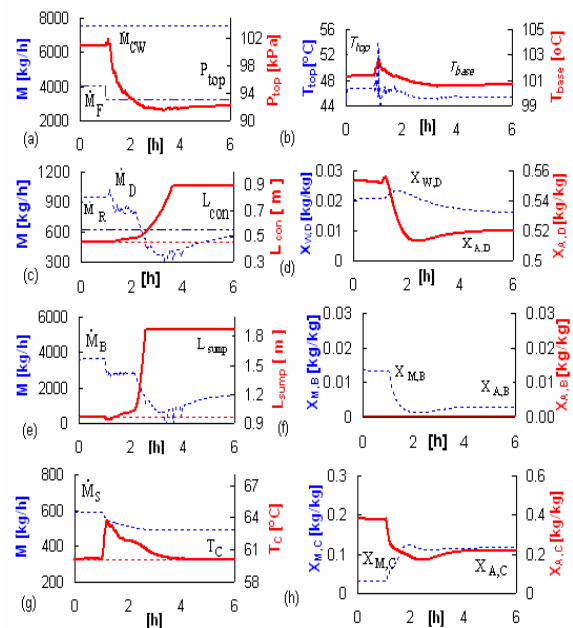


Figure 4. Dynamic simulation results for disturbance of step down change of 20 % in feed rate 3.1. Step down change of 20% in feed rate.

#### 4. Process Disturbance Simulation for Operational Failures

The physical effects and risk related consequences of the operational failures are analyzed by disturbance simulation. It is not possible to simulate the operational failures such as foaming, fouling, rupture of pipe etc. with commercial simulation tools like Aspen dynamics or dynamic simulation models. However, simulation of scenarios of increase / decrease in parameters like steam flow rate, feed flow rate, reflux flow etc. can be simulated for safety examination (by giving large disturbances). Thus, following scenarios are simulated:

1. Too less cooling capacity

- Step down change of 30 % in cooling medium flow (i.e from 7590 to 5313 kg/h)
  - Step down change of 50% in cooling medium flow (i.e. from 7590 to 3795 kg/h)
2. Total loss of cooling medium flow

These disturbances are introduced by step change.

3. Step up change of 20% in steam flow rate (589 kg/h to 707 kg/h) --- this disturbance is introduced by step change and removing temperature controller (assuming failure of temperature controller).
4. Maximum feed flow considering feed pump capacity (4021 kg/h to 5239 kg/h) --- this disturbance is introduced by step up change and removing feed flow rate controller (assuming failure of feed controller).
5. Step up change of 50% in reflux flow (619 kg/h to 938 kg/h)
6. Restriction/blockage of vent line plus pressure rise --- this disturbance is simulated by closed column under atmospheric pressure with various levels of failure of cooling medium flow
7. Step up change of 20 % in cooling medium flow (7590 kg/h to 9108 kg/h) --- this disturbance is introduced by step change.
8. Step down change of 50% in reflux rate (619 kg/h to 309 kg/h).

These scenarios are first simulated with existing control scheme. Then, keeping in view the strict environmental constraints, control tray temperature is changed from tray 8 to tray 24 and same scenarios are simulated again. Next, the dual composition control configuration (i.e. reflux flow is controlled by the temperature of tray 8 and steam flow is controlled by temperature of tray 24) is also examined by simulating the same scenarios. However disturbance simulation results of only scenario (1) and (2) are described here and details of other scenarios can be found somewhere else [6].

#### 4.1. Step down change of 30 % in cooling medium flow

Figure 5 (a-h) shows the response of column and control behaviour of simulation model with control temperature tray 8 for step down change of 30 % in cooling medium flow. At simulation time  $t =$

1 h, a step change in the cooling water flow rate from 7590 to 5313 kg/h is introduced. At the introduction of this disturbance, the column top pressure starts increasing from the set point 101.036 kPa (atmospheric pressure) due to accumulation of vapours (see figure 5 a). This increase leads to increase of column top and base temperature as well (see figure 5b). As the pressure becomes just high than atmospheric pressure, pressure relief valve opens to release the vapour to atmosphere to avoid high pressure. Figure 5 (g) shows that the rate of material released to atmosphere reaches upto 366 kg/h in order to avoid overpressure. The released material may or may not dispersed safely depending upon the environmental conditions and geographical location. The release of material may result into a range of possible incident outcomes such as jet fire, vapour cloud explosion (VCE) and flash fire. The column top pressure stabilizes at 101.5 kPa (see figure 5 a). Due to release of vapour in the atmosphere and constant reflux flow, the liquid level in the reflux drum falls down from the set point (see figure 5 c). The level controller works and distillate flow rate falls down (from 951 to 587 kg/h) in order to bring the liquid level back to the set point (see figure 5 c). Figure 5 (d) & (f) shows that column head and base product quality do not disturb and remains within the targets. The dynamic behavior of the column with control tray 24 and dual composition control is similar as in the case of column with control tray 8 for this disturbance.

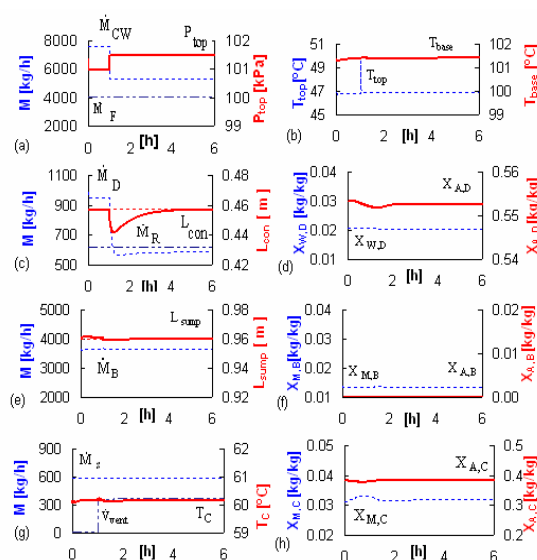


Figure 5. Disturbance simulation results for step down change of 30% in cooling medium flow for control tray 8.

4.2. Step down change of 50 % in cooling medium flow

Figure 6 (a-h) shows the response of column and control behavior of simulation model with control temperature tray 8 for step down change of 50 % in cooling medium flow. The dynamic behaviour of the column is similar as for 30 % loss of cooling medium flow but with high magnitude of order. The pressure rises from atmosphere and stabilizes at 102.4 kPa (see figure 6a).

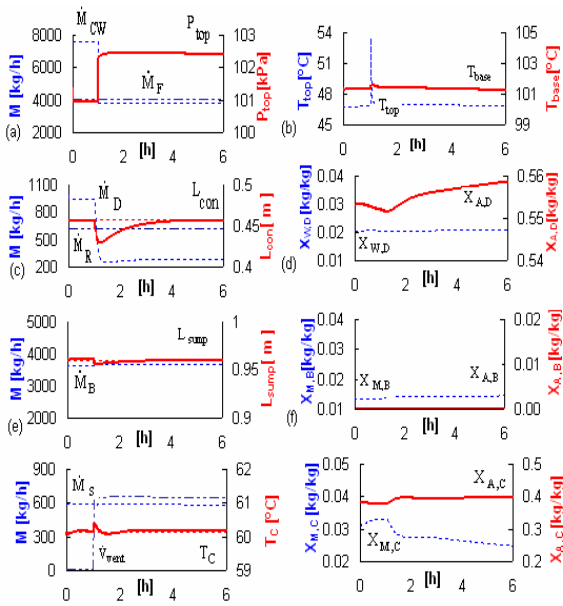


Figure 6. Disturbance simulation results for step down change of 50% in cooling medium flow for control tray 8

The amount of material released (651 kg/h) to atmosphere becomes approximately double as compared to 30 % loss of cooling (see figure 6 g). The distillate flow reduces to 288 kg/h (see figure 6 c). All controllers work satisfactorily (see figure 6 c, e & g) and product quality remains within purity targets (see figure 6 d & f). The dynamic behavior of the column with control tray 24 and dual composition control is also found similar as in the case of column with control tray 8.

4.3. Total loss of cooling

The behavior of the column is entirely different in case of very large disturbance such as total loss of cooling medium flow. Figure 7(a-h) shows the dynamic response of simulation model with control temperature tray 8 for total loss of cooling medium flow. At simulation  $t = 1$  h, the disturbance of no flow of cooling water is introduced by step change

(see figure 7 a). The pressure of the column rises sharply (upto 111 kPa) at the introduction of this disturbance (see figure 7a). This give rise to column temperature profile within the column as column top temperature increases to approximately 71 °C and column base temperature also increases to 104 °C (see figure 7 b). The temperature of control tray also increases. To bring the control tray temperature back to its set point, the steam flow rate decrease (see figure 7 g). To avoid the dangerous situation of overpressure the process relief valve opens completely and the rate of material released becomes approximately (1600 to 1800) kg/h (see figure 7 g). As pressure driven simulation is carried out so the increase of column pressure results in loss of feed flow rate therefore the distillate flow, reflux and base product flow falls to zero (see figure 7 a, c & e). Therefore, in about 45 minutes of simulation time after introducing the disturbance, the simulation stops. In real plant, a pump is installed after reflux drum for providing energy for distillate and reflux flow. So distillate and reflux flow falls to zero because after some time liquid level in reflux drum falls down and it filled with vapours.

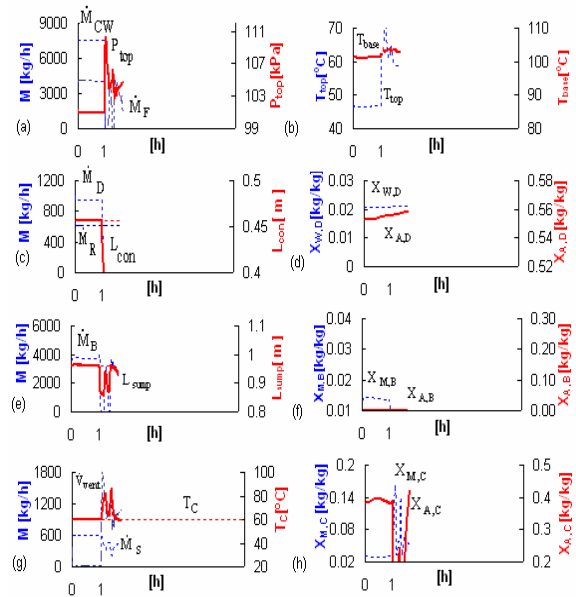


Figure 7. Disturbance simulation results for total loss of cooling for control tray 8.

The dynamic response of simulation model with control temperature tray 24 for total loss of cooling medium flow is similar as for column with control tray temperature 8 with the only difference in magnitude of increase in top temperature is more

(i.e. rise up to 85 °C instead of 71 °C). The dynamic response of simulation model with dual composition control for total loss of cooling medium flow similar as in previous cases.

## 5. Conclusion

After analyzing the results and due to increasing strict environmental regulations, the control tray temperature is modified from tray 8 to tray 24 in order to improve the effluent quality. The following risk related consequences are expected to occur in case of these failure scenarios 1) Product quality deterioration, 2) Loss of production, 3) Release of material which may or may not safely dispersed.

## Nomenclature

No.	Variables	Symbols
1	Cooling water flow rate [kg/h]	$\dot{M}_{CW}$
2	Feed flow rate [kg/h]	$\dot{M}_F$
3	Column head pressure [kPa]	$P_{top}$
4	Column head temperature [°C]	$T_{top}$
5	Column base temperature [°C]	$T_{base}$
6	Distillate flow rate [kg/h]	$\dot{M}_D$
7	Reflux flow rate [kg/h]	$\dot{M}_R$
8	Condenser liquid level [m]	$L_{con}$
9	Water mass fraction in distillate [kg/kg]	$X_{W,D}$
10	Acetone mass fraction in distillate [kg/kg]	$X_{A,D}$
11	Base flow rate [kg/h]	$\dot{M}_B$
12	Sump level [m]	$L_{sump}$
13	Acetone mass fraction in base [kg/kg]	$X_{A,B}$
14	Methanol mass fraction in base [kg/kg]	$X_{M,B}$
15	Steam flow rate [kg/h]	$\dot{M}_S$
16	Control tray temperature [°C]	$T_C$
17	Vent flow rate [kg/h]	$\dot{V}_{vent}$
18	Acetone mass fraction at control tray [kg/kg]	$X_{A,C}$
19	Methanol mass fraction at control tray [kg/kg]	$X_{M,C}$

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