Lecture Notes in Networks and Systems 1091

Volodymyr Kazymyr · Anatoliy Morozov · Alexander Palagin · Serhiy Shkarlet · Nikolai Stoianov · Dmitri Vinnikov · Mark Zheleznyak *Editors*

Mathematical Modeling and Simulation of Systems

Selected Papers of 18th International Conference, MODS, November 13–15, 2023, Chernihiv, Ukraine

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Preface

The International Conference "Mathematical Modeling and Simulation of Systems" (MODS) was formed to bring together outstanding researchers and practitioners in the field of mathematical modeling and simulation from all over the world to share their experience and expertise.

The conference MODS was established by the Institute of Mathematical Machines and Systems Problems of the National Academy of Sciences of Ukraine (NASU) in 2006. MODS is now an annual international conference held by Chernihiv Polytechnic National University with the assistance of the Ministry of Education and Science of Ukraine, the NASU and the State Research Institute for Testing and Certification of Arms and Military Equipment, universities and research organizations from UK, Japan, Sweden, Bulgaria, Poland, Estonia, and Ukraine participating as co-organizers of the conference.

The 18th International Conference MODS'2023 was held in Chernihiv, Ukraine, during November 13–15, 2023. MODS'2023 received 59 paper submissions from different countries. All papers went through a rigorous peer-review procedure including pre-review and formal review. Based on the review reports, the Program Committee finally selected 30 high-quality papers for presentation on Conference sessions, which are included in "Lecture Notes in Networks and Systems" series.

This book contains papers devoted to relevant topics including tools and methods of mathematical modeling and simulation in ecology and environment, manufacturing and energetics, information technology, modeling, analysis, and tools of safety in distributed information systems, mathematical modeling and simulation of special purpose equipment samples, and cyber-physical systems. All of these offer us plenty of valuable information and would be of great benefit to the experience exchange among scientists in modeling and simulation.

The organizers of MODS'2023 made great efforts to ensure the success of this Conference despite the active military operations on the territory of Ukraine. We hereby would like to thank all the members of MODS'2023 Advisory Committee for their guidance and advice, the members of Program Committee and Organizing Committee, and the referees for their effort in reviewing and soliciting the papers, and all authors for their contribution to the formation of a common intellectual environment for solving relevant scientific problems.

Also, we are grateful to Springer-Verlag and Janusz Kacprzyk as the editor responsible for the series “Lecture Notes in Networks and Systems” for their great support in publishing these selected papers.

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Mathematical Modeling and Simulation of Systems in Ecology

Combining HAZOP Technique and Modeling of High-Energy Processes in Reflux Drum of Hydrocarbons Distillation Process as an Element of Process Safety Information Technology

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Abstract. Standard method of hazard identification HAZOP has several limitations: impossibility to identify hazards involving interactions between different parts of complex system; experts' experience can fail while evaluating deviations of process parameters, their causes and consequences; it is nearly impossible to conduct manual calculations due to limited time for HAZOP session. These limitations can be potentially solved using quantitative risk analysis and assessment information technologies. The idea is to combine HAZOP study and mathematical modeling of an element of chemical technology system. So, the model of process tank has been developed. Reflux drum of hydrocarbon stabilizing fractionating column of the isomerization unit has been chosen as the object of study. Numerical experiment has shown that standard HAZOP study (without modeling) provided greatly overestimated conclusion about the possibility of reflux drum depressurization. Standard HAZOP suffers of significant lack of data about process deviations and dangerous conditions of equipment. Only modeling of process parameters deviations can give sufficient information for hazard identification and further quantitative risk assessment of process equipment depressurization.

Keywords: hazard identification · HAZOP · risk analysis · risk assessment · dynamic modelling · phase equilibrium · hydrocarbons · process tank · reflux drum

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1 Introduction

To be able to manage safety using Risk-Based Approach (RBA) for all potentially dangerous facilities in Ukraine it is necessary to assess the level of risk using qualitative or quantitative methods of analysis and assessment. A transition from dominant 100% security paradigm to the RBA requires significant amount of efforts that are necessary to cope with multiple engineering tasks during each stage of RBA. However due to development of modern information technologies for quantitative risk analysis & assessment it is possible to save both state and private enterprises' budgets via significant reducing of time and cost for risk assessment procedures [1].

Hazard identification is an important step in risk management processes. Usually this stage is performed by experts; modern standards, including international ones (IEC 31010:2019), recommend using the following methods: checklists, FME(C)A, HAZOP, Scenario Analysis, SWIFT [2].

HAZard and OPerability Study (HAZOP) is one of the best and most rigorous methods for identifying hazards and performance issues of chemical facility. HAZOP procedure formally examines, using specific guide words, every process equipment, as well as deviations from its normal operating conditions, and considers possible malfunctions. HAZOP report includes all deviations, causes, consequences of process parameters, analysis of such consequences, implemented safety instrumented systems (active and/or passive) and final proposals [3].

HAZOP requires many hours of work by a team of experienced engineers, and it is not easy to record (and formalize) engineering reasoning, basic input information or results [3]. For complex technological systems, the danger of deviation of process parameters in equipment cannot be unambiguously identified even by a group of experienced specialists without calculations. Therefore, to overcome uncertainty, a conservative estimate is usually adopted, which sometimes leads to significant excess costs to reduce the risk to acceptable level.

Thus, it is impossible to carry out quantitative risk assessment by an expert within affordable time without the use of modern information technologies that make it possible to simulate complex technological systems with accuracy of mathematical model [1].

Study shows that to overcome disadvantages of standard HAZOP technique two types of informational technologies have been developed. The first one is a typical expert approach [4, 5], which usually consists of several knowledge databases. The second one is more advanced model-based approach [3, 6] that has gained more importance in the last years. It offers an opportunity to describe chemical plant via mathematical modeling. Model-based approach allows to:

- minimize human factors,
- perfectly formalize deviations of process parameters;
- provides necessary data for further consequences assessment.

Though existing methods [7, 8] greatly focus on studying of the deviation of process parameters inside of equipment, they do not consider criteria for achieving such a state that leads to depressurization. They also don't provide a set of parameters that is necessary to assess the consequences of depressurization.

With advanced development of computer technologies, such a way of combining process modeling and HAZOP, that allows to obtain all the necessary information about depressurization state, in our opinion, is a positive vector for the development of systematic approach in risk analysis and assessment.

The aim of this research is to create a relatively simple mathematical model of process tank, taking into account the heat and mass transfer processes occurring in it. The model should be applicable for information technology of risk analysis during the HAZOP study. Safety experts should be allowed to specify deviations of process parameters from the project intent and identify those deviations that can lead either to accidental depressurization or to disruptions in technological process causing significant financial losses.

The model should predict the behavior of main state parameters of chemical system that are necessary to assess the occurrence of a dangerous state inside the equipment (process tank) which is leading to depressurization.

Considering an opportunity for integration of the model in information technology for predicting the consequences of an emergency releases, it is necessary to take into account the possibility of multicomponent composition of the chemical system inside the apparatus. This is important for many modern phenomenological models for predicting release rate of hazardous substance into the atmosphere, for example, for the evaporation of an emergency spill of multicomponent liquid phase [9].

2 Mathematical Model Description

The model of high-energy phenomena in process tank is deterministic, dynamic model and allows to determine the parameters of the state of a two-phase system for the mixture of substances inside the tank at any moment of modeling time (Fig. 1).

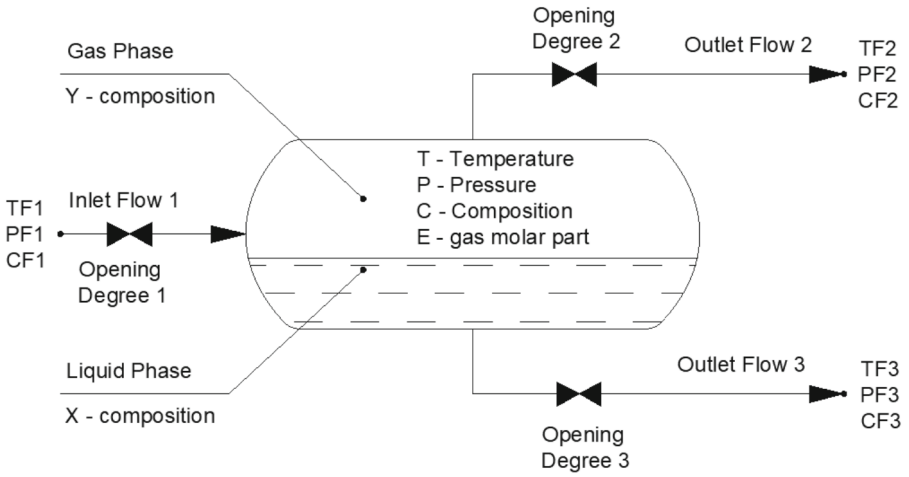

Fig. 1. Schematic description of process tank with inlet and outlet flows

Let's make considerations which are common for chemical technologies:

- process tank – a hollow, thermally insulated thin-walled object, which is characterized by volume V [m^3] and size (shape);
- there is a mixture of substances inside of process tank that forms a single-phase or two-phase equilibrium system (Fig. 1);
- the system inside of process tank is characterized by state parameters: temperature T [K], vapor phase pressure P [Pa], volume equal to the volume of the tank V, composition vector of the vapor-liquid mixture C [molar parts] and molar part of the vapor phase E (Fig. 1);
- n streams are connected to process tank; streams can be both inlet and outlet and are characterized by composition vectors CF1-CFn [molar parts], temperatures TF1-TFn, external pressure (pressure) PF1-PFn, as well as resistance coefficients, diameters and degrees of control valves opening (Fig. 1);
- each stream is equipped with backflow prevention device that prevents the backflow of the substance.

The temperature dependences of saturated vapor pressure and liquid phase density for each component of the system are known [10].

Phase equilibrium for ideal multiphase mixture can be described using Rachford-Rice equation [11, 12]:

$$\sum_{i=1}^{nsubst} \frac{C_i(k_i - 1)}{1 + E \cdot (k_i - 1)} = 0 \tag{1}$$

where:

- *nsubst* – is a number of components of the mixture;
- C_i – composition [molar parts] of multiphase mixture inside of process tank;
- k_i – distribution coefficient;
- E – is the molar part of the vapor phase.

Distribution coefficients are determined as:

$$k_i = \frac{p_i^0(T)}{P} \tag{2}$$

where:

- $p_i^0(T)$ (T) is the pressure [Pa] of the saturated vapor of the i-th component at the temperature T [13].

By solving Eq. (1) it is possible to determine the molar part of vapor E at specified temperature, pressure and mixture composition, using, for example, Newton-Raphson method or the bisection method.

Molar volume of the mixture inside of process tank (accounting molar part E of the gas phase) is determined as:

$$V_M = E\frac{RT}{P} + (1-E)\sum_{i=1}^{nsubst}\frac{X_i \cdot M_i}{\rho_i(T)} \tag{3}$$

where:

- E – gas molar part;
- R – gas constant 8.314 [J/(mol·K)];
- X_i – temperature inside of process tank;
- M_i – molar mass [kg/mol] of the i-th component;
- $\rho_i(T)$ – density [kg/m^3] of the i-th component at temperature T.

Molar fractions X_i of components in liquid phase are determined such as:

$$X_i = \frac{C_i}{1 + E \cdot (k_i - 1)} \tag{4}$$

Molar fractions Y_i of components in gas phase are determined such as:

$$Y_i = \frac{C_i k_i}{1 + E \cdot (k_i - 1)} \tag{5}$$

The equation of matter conservation in differential form:

$$\frac{\mathrm{d}N_\Sigma}{\mathrm{d}\tau} = \sum_{\mathrm{i}=1}^{\mathrm{l}} \mathrm{F}_{income,\mathrm{i}} - \sum_{\mathrm{j}=1}^{\mathrm{m}} \mathrm{F}_{outcome,\mathrm{j}} \tag{6}$$

where:

- l – the number of flows into process tank;
- m – the number of flows out of process tank;
- N_Σ – amount [mol] of multiphase mixture inside of process tank;
- $\mathrm{F}_{income,\mathrm{i}}$ – i-th flow rate [mol/s] through the pipe into process tank;
- $\mathrm{F}_{outcome,\mathrm{j}}$ – j-th flow rate [mol/s] through the pipe out of process tank.

Flows' rates could be evaluated via well-known equations e.g. Bernoulli equation. Opening degree of each control valve and pipeline resistance coefficients should be taken into consideration.

The equation of matter conservation for each chemical component could be written as:

$$\frac{\mathrm{d}(N_\Sigma \cdot \mathrm{C_s})}{\mathrm{d}\tau} = \sum_{\mathrm{i}=1}^{\mathrm{l}} \left(\mathrm{F}_{income,\mathrm{i}} \cdot \mathrm{C}_{\mathrm{F\_inc_{i,s}}}\right) - \sum_{\mathrm{j}=1}^{\mathrm{m}} \left(\mathrm{F}_{outcome,\mathrm{j}} \cdot \mathrm{C}_{\mathrm{F\_out_{j,s}}}\right) \tag{7}$$

where:

- $\mathrm{C_s}$ – molar concentration of the s-th component in vapor-liquid mixture;
- $\mathrm{C}_{\mathrm{F\_inc_{i,s}}}$ – molar part of the s-th component in the i-th flow entering process tank;
- $\mathrm{C}_{\mathrm{F\_out_{j,s}}}$ – molar part of the s-th component in the j-th flow leaving process tank.

The equation of heat conservation:

$$\frac{\mathrm{dH}}{\mathrm{d}\tau} = \sum_{\mathrm{i}=1}^{l} \left(\mathrm{F}_{income,\mathrm{i}} \cdot h_{F\_inc_i}\right) - \sum_{\mathrm{j}=1}^{\mathrm{m}} \left(\mathrm{F}_{outcome,\mathrm{j}} \cdot h_{F\_out_j}\right) \tag{8}$$

where:

- $h_{F\_inc_i}$ – molar enthalpy [J/mol] of the i-th flow entering into process tank;
- $h_{F\_out_j}$ – molar enthalpy [J/mol] of the j-th flow coming out from process tank.

ODE system (6, 7 and 8) is supposed to be solved via iterative methods. It is recommended to use the 4-th order Runge-Kutta method with auto correction of the step [14]. In case of computation slowdown, Euler methods (explicit/implicit) can be used cautiously [15].

After obtaining substance amount $N_{\Sigma,\tau+\Delta\tau}$ and total mixture enthalpy $\mathrm{H}_{\tau+\Delta\tau}$ for the next time step, we determine molar volume $V_{M,\tau+\Delta\tau}$ and molar enthalpy $h_{\Sigma,\tau+\Delta\tau}$ of the mixture for the next moment of modeling time.

On the other hand, molar enthalpy of two-phase mixture is determined as:

$$h_\Sigma = (1-E)\sum_{i=1}^{nsubst}(h_{l_i}(T)\cdot X_i) + E\sum_{i=1}^{nsubst}\left(h_{g_i}(T)\cdot Y_i\right) \tag{9}$$

Equations (3) and (9) form a system of non-linear equations with two unknowns that should be found: $T_{\tau+\Delta\tau}$ and $P_{\tau+\Delta\tau}$ (considering E, X and Y as a function of $T_{\tau+\Delta\tau}$ and $P_{\tau+\Delta\tau}$ as well):

$$\begin{cases} V_{M,\tau+\Delta\tau} = E\frac{RT_{\tau+\Delta\tau}}{P_{\tau+\Delta\tau}} + (1-E)\sum_{i=1}^{nsubst}\frac{X_i\cdot M_i}{\rho_i(T_{\tau+\Delta\tau})} \\ h_{\Sigma,\tau+\Delta\tau} = (1-E)\sum_{i=1}^{nsubst}(h_{l_i}(T_{\tau+\Delta\tau})\cdot X_i) + E\sum_{i=1}^{nsubst}\left(h_{g_i}(T_{\tau+\Delta\tau})\cdot Y_i\right) \end{cases} \tag{10}$$

After solution of the system (10), algorithm cycles again for the next time step.

Main output parameters of process tank model are:

- T – temperature [K] of the mixture in process tank for each moment of modeling time;
- P – pressure [Pa] inside of process tank for each moment of modeling time;
- X, Y – vectors of equilibrium compositions [molar parts] of the liquid and vapor phases respectively (for every moment of modeling time);
- E – molar part of gas phase for every moment of modeling time;
- N – amount [mol] of substance inside of process tank for every moment of modeling time.

Based on mathematical description of the model, an algorithm has been developed for calculating of numerical parameters of high-energy processes inside of storage tank.

For process tank (regardless of its configuration) the design pressure is known, which is determined with a margin. For any vessel, regardless of its geometry, hydraulic test pressure is usually equal to 1.25 of design pressure with some amendments and exceptions. The pressure and temperature (for dangerous state) at which deformation begins are usually significantly higher.

In the case of absence of passport data for process tank design pressure, an assessment of rupture pressure can be estimated (for horizontal cylinder as shown on Fig. 1) via following formula [16]:

$$P_{burst} = 2\sigma_u \cdot \frac{W}{D_t} \tag{11}$$

where:

- W – process tank wall thickness;
- D_t – tank diameter;
- σ_u – ultimate strength at the temperature of the tank wall.

3 Numerical Experiment Description

Reflux drum T-5 of stabilizing fractionating column C-3 of the isomerization unit has been chosen as the object of study (Fig. 2). The upper product of the C-3 stabilization column is cooled in the air cooler AC 1–3 and then in water cooler WCC 1. After cooling the flow enters reflux drum T-5 (Fig. 2).

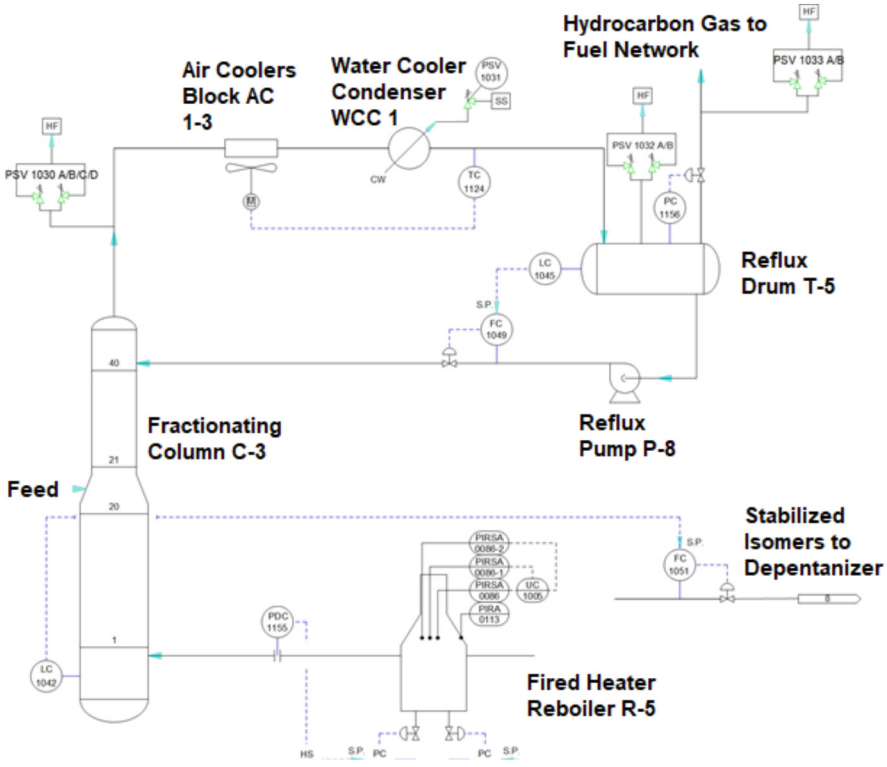

Fig. 2. P&ID of the process of stabilization of the isomerization unit [17]

In the reflux drum T-5 hydrocarbon gas is separated from the liquid phase.

Table 1. Design intent process parameters for reflux drum T-5

Name of process stage, equipment, state controllers	State controller position number on the P&ID	Measuring units	Permissible limits of technological parameters	Required accuracy class of measuring instruments
Pipeline 100. Flow rate of hydrocarbon gas from T-5 into fuel network	FQIR 1048	m^3/h at standard pressure and temperature	1180 ÷ 3500	1.0%
Process Tank T-5. Liquefied gas level	LIRCA 1045	% range	25 ÷ 75	1.0%
Pipeline 100. Hydrocarbon gas pressure in fuel network	PI 1210	MPa	No more than 0.737	0.5%
Process Tank T-5. Pressure in T-5	PIRCA 1156	MPa	1.511 ÷ 1.550	0.5%
Pipeline 100. Temperature of hydrocarbon gas out of T-5 into fuel network	TI 1249	°C	30 ÷ 40	1.0%

Table 2. Technical parameters of T-5

Design temperature, °C	Design pressure, MPa	Diameter, m	Length, m
120	1.9	2.4	7.2

Hydrocarbon gas is then sent to fuel network. Liquefied gas from reflux drum T-5 is supplied by pump P-8 as reflux to the stabilization column C-3. Design intent process parameters for T-5 are given in Table 1. Technical parameters of reflux drum T-5 are given in Table 2.

Table 3. HAZOP study of T-5, [18]

Process parameter – GUIDE WORD	Causes	Deviation	Consequences	Protection Mechanisms
Pressure – MORE	Pressure increasing in T-5 due to malfunction of cooling system AC 1–3, WCC 1	Pressure is more than 1.6 MPa in T-5	*Safety:* T-5 rupture, dangerous substance release, fire, explosion *Ecology:* Environmental Pollution *Exploitation:* Production interruption	PRV: PSV 1032AB; Control: PIRC 1156

HAZOP procedure has been carried out using brainstorming according to [18]. For simplicity, we will consider only one row of the HAZOP table, leading to depressurization (Table 3).

However, HAZOP data (Table 3) does not contain information necessary and sufficient to quantitatively estimate the consequences of the accident. It is only known that the pressure in the apparatus has exceeded 1.6 MPa, but it is unknown what is the temperature, amount and composition of the mixture inside of reflux drum at the moment of rupture. In the order to eliminate the uncertainty about state parameters inside of reflux drum, a computational experiment has been carried out according to the developed process tank model.

4 Results and Discussion

The behavior of state parameters inside of T-5 reflux drum has been modeled for non-standard process conditions due to the failure of cooling units. According to the design intent, the temperature of the top of the column is 368 K. In order to prevent underestimation of potential hazard, the temperature of the top of the column has been considered to be equal to 400 K. Thus, in the event of a failure of the cooling system, a mixture with a temperature of 400 K will enter the reflux drum so higher internal pressure could be achieved inside of T-5. Initial state parameters inside of reflux drum are:

- Pressure – 1511000 Pa;
- Temperature – 308 K;
- Gas phase molar part – 0.462.