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Development and creation a model of a digital twin of the cubepart rectification installation for the separation of a binary water-alcohol mixture

R A Khakimov and N S Shcherbo

Faculty of Magistracy and Elite Education Omsk state technical university, 644050, Omsk, Pr. Mira, 11, Russia

Abstract. In article the way of creation of development of the digital twin of a cube part of a rectification column for the separation of a binary water-alcohol mixture, using the software Matlab/Simulink is considered. The technology solution on creation and verification of the digital twin of the available laboratory installation and structure of digital model, which is the basis for the digital twin, are developed.

1. Introduction

As part of the piecemeal oncoming Industry 4.0, digital twins are one of the main elements on which the industry will begin its development. Therefore, now many leading engineering collectives and laboratories are engaged in creation and development of digital twins, and, achievements in the field of digital modeling, even have experience of introduction on productions abroad, mainly, at oil refineries.

Basis of simulars of technological process are the general principles of calculations of material - thermic balances of oil processing productions (productions, connected with change of aggregate state and also the component and chemical composition of material streams concern them).Each production consists of several stages, each of which converts energy and produces a certain effect on material flows. Technological schemes are usually used to describe the sequence of stages, where each element corresponds to a specific technological process.Connections between elements in technological schemes represent material and power streams. As the basis of Modeling of the technological scheme is used the general principles of thermodynamics, both to separate elements of the scheme, and to system in general.

2. Problem definition

The purpose of work is creation of the digital twin of the existing laboratory installation of a rectifying column for division of binary mix. And also a research of a technique of creation of such doubles for her further use in creation of other digital models. For achievement of this purpose it is required to solve a number of problems, such as research of laboratory installation; creation of the digital twin of installation in the modeling environment; verification and assessment of accuracy of work of the double.

3. Theory

Rectification of ethanol - the containing mix is carried out by means of laboratory to rectifying installation (figure 1). As a heating element the tiny tile is used. Process of rectification happens to periodic refueling of ethanol-containing raw materials. Installation comprises three main parts — a evaporative cube, the mass-exchanged section, filled with a nozzle and the condenser.

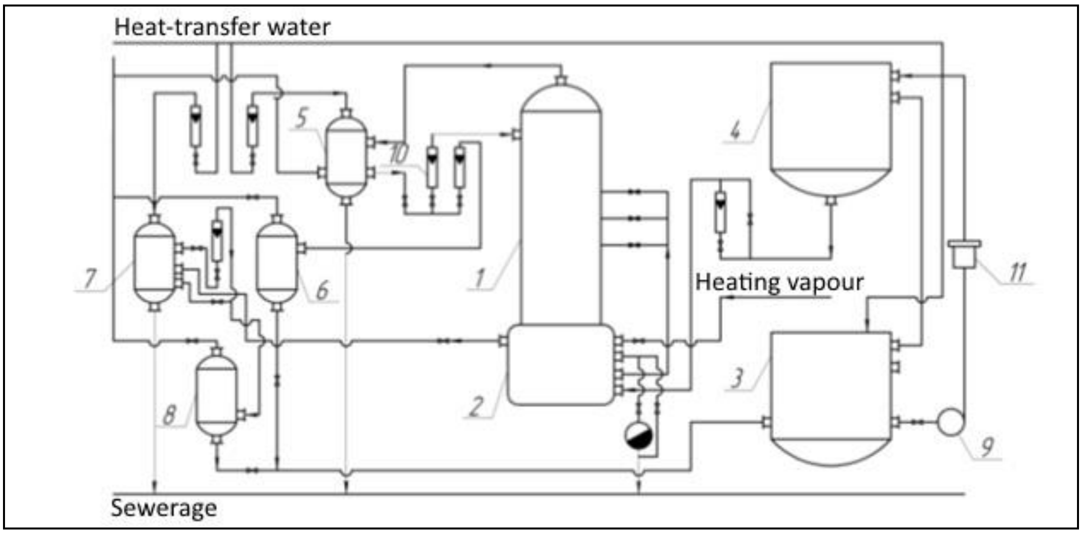

Figure 1. Schematic diagram of laboratory installation.

The main part of installation is the compound column consisting from top and lower rectifying parts. Conditionally, the top part includes the condenser, the refrigerator for condensation of the selected mix, the alcohol selection regulator and also the system of binding branch pipes. At rectification in the refrigerator and the condenser executed according to the scheme "pipe in a pipe", constantly a countercurrent reverse water which creates necessary outflow of heat from mix arrives. In the top part of vat capacity conclusions of a manometrical tube are drawn.

During the experiment, concentration of the received alcohol is determined by the current values of its density (static pressure of a calibrated column of the liquid which is taken away in alcohol receiver taking into account her temperature). Key parameters of work of a column, such as temperature, pressure, content of alcohol in the selecting mix are registered by means of a set of the sensors installed in a column and operated by the computer.

First of all, it is necessary to determine a set of independent parameters and indicators on the basis of which the model will work. Among such parameters:

- Operating mode of the heater, in Watts;
- The volume and composition of the mix which is filled in in a cube;
- Reference temperature of the liquid which is filled in in a cube;
- Sizes and form of a cube;
- Air temperature.

The main control parameters are indicators poured into the mixture container and the power of the heater as they can be changed freely before start of a column for verification of model.

In general, the obtained experimental data of work of installation show that pressure cubed of a column increases slightly. Therefore, the decision not to consider influence of change of pressure upon some dependent parameters, such as specific heat of steam formation or coefficients of a thermolysis has been made. Therefore, a state equation role in this model - creation of curve dependence of pressure from time is exclusive, according to this task the equation was chosen.

Based on the relevant literature on heat transfer, a model was created, shown in figure 2.

In the beginning, during the analysis the decision to use the cubic equation of Peng-Robinson which well proved to be when modeling vapor-liquid balance and calculating density of liquid of hydrocarbonic systems has been made. However, this equation in case of its application to nonideal systems which alcohol-containing mix is, yielded too inexact results. Therefore, instead of the original cubic equation of Peng-Robinson it has been decided to use his modification offered by Strizheck and

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Vera in 1986. This modification extended application of an initial method to nonideal systems. Also this equation corresponds to curves of elasticity of vapors of clean components and mixes much more precisely and has more flexible rule of mixture. [12,13]

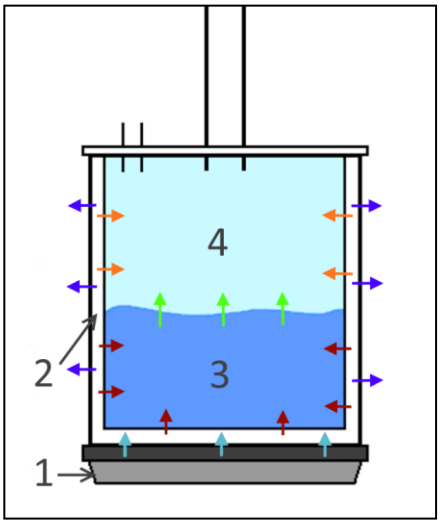

Figure 2. Model of distribution of thermal streams in a cube part of a column. 1 - A heating tile, 2 - cube Material, 3 - Mix of ethanol and water, 4 - Steam-gas mix.

Modification of the equation of a condition of Peng-Robinson has been offered in 1986 by scientists Strizhek and Vera. This cubic equation of a state which for brevity has the designation PRSV has one additional adjustable parameter for clean connection. Using suitable two-parametrical rules of mixture this equation can be used for reproduction of data on balance of steam and liquid mix with accuracy, comparable with some general double methods in which activity coefficients for a liquid phase and also the special equations of a state for a steam phase are used. Subsequently, additional modification of the created PRSV of the equation which reflected processes of unideal systems even more precisely has been offered.

The recent research has also shown that the values of fugitives calculated from the equation of PRSV reflect a real PVT picture in vapor-liquid system most precisely, even more precisely than the data obtained by dual methods. [14]

PRSV modification of the equation of a state formally corresponds to the equation offered by Peng and Robinson in 1976:

$$P = \frac{R \cdot T}{V - b} - \frac{a \cdot \alpha}{V^2 + 2 \cdot b \cdot V - b^2} \quad (1)$$

where P — pressure of saturated steam in system; T — temperature in system; V \molar volume; andα and b — the special coefficients calculated on the following formulas:

$$a = 0.457235 \cdot \frac{R^2 \cdot T^2}{Pc} \quad (2)$$

$$\alpha = (1 + k \cdot (1 - T_R^{0.5}))^2 \quad (3)$$

$$b = 0.077796 \cdot \frac{R \cdot T_c}{Pc} \quad (4)$$

The way of calculation of coefficient of k for further calculation of parameter α in the equation was the main change offered within PRSV of modification (4.10):

$$k = k_0 + k_1 \cdot (1 + T_R^{0.5}) \cdot (0.7 - T_R) \quad (5)$$

where

$$k_0 = 0.378893 + 1.489715 \cdot \omega - 0.1713848 \cdot \omega^2 + 0.0196544 \cdot \omega^3 \quad (6)$$

And in the equation (6) the k0 parameter is called Single Pure Compound Adjustable Paramter. The k0 value depends on critical values of temperature Tc and pressure of Pc and also on an acentric factor ω which are individual for each parameter of mix.

The given formulas (1) — (6) are fair only for the clean systems consisting of one component. For the systems containing two and more components it is necessary to use Wang-der-Vaals rules of mixture for difficult systems. For work with difficult systems first of all it is necessary to transform the equation (1) to a polynomial appearance:

$$z^3 - (1 - B) \cdot z^2 + (A - 3B^2 - 2B) \cdot z \\ -(A \cdot B - B^2 - B^3) = 0 \tag{7}$$

Where

$$z = \frac{P \cdot V}{R \cdot T} \tag{8}$$

$$A = a \cdot \alpha \frac{P}{\cdot R^2 \cdot T^2} \tag{9}$$

$$B = b \cdot \frac{P}{R \cdot T} \tag{10}$$

Rules of mixture for parameters in multicomponent systems have the following appearance:

$$a\alpha = \sum \sum y_i y_j (a\alpha)_{ij} \tag{11}$$

$$b = \sum y_i b_i \tag{12}$$

$$(a\alpha)_{ij} = (1 - k_{ij}) \cdot \sqrt{(a\alpha)_i \cdot (a\alpha)_j} \tag{13}$$

$$A = \sum \sum y_i y_j A_{ij} \tag{14}$$

$$B = \sum y_i B_i \tag{15}$$

$$A_{ij} = (1 - k_{ij}) \cdot \sqrt{A_i \cdot A_j} \tag{16}$$

In the used equations of k_{ij} is a coefficient of binary interaction between i and j component; y_i is a molar maintenance of a component in mix. [14,15,16]

The mathematical model offered for use which will be created in a Matlab/Simulink package is guided by the basic fundamental laws and the equations which describe behavior of binary mix cubed of a column. The full graphic type of mathematical model is presented in the figure 3, it reflects not only conditional division of model into separate blocks of processing of various data, but also shows interrelations between these blocks. On this basis the digital model of a cube which will be verified by real data of his work will be created, and, on the basis of this verification the result whether it is possible to consider the created model the digital double will be summed up.

4. Results of an experiment

Following the results of work, the model creates three schedules of dependences of Pressure, Temperature of liquid and temperature in gas area of a cube. These data remain in the form of special objects of Simulink library then are in a special way processed and verified (figure B1). Verification of model on experimental data happens in the same graphic coordinates, and it is possible to judge reliability of the digital twin in process of coincidence of data of his work with the schedule of real work of a column. At the same time, because of not ideality of the registering devices it is required to make linearization of basic graphic data for experimental data in the beginning. As a linearization technique for data the way of nonlinear regression of the eighth order (Non-linearregression 8thgrade) as he most precisely reflects average value on an experiment has been chosen.

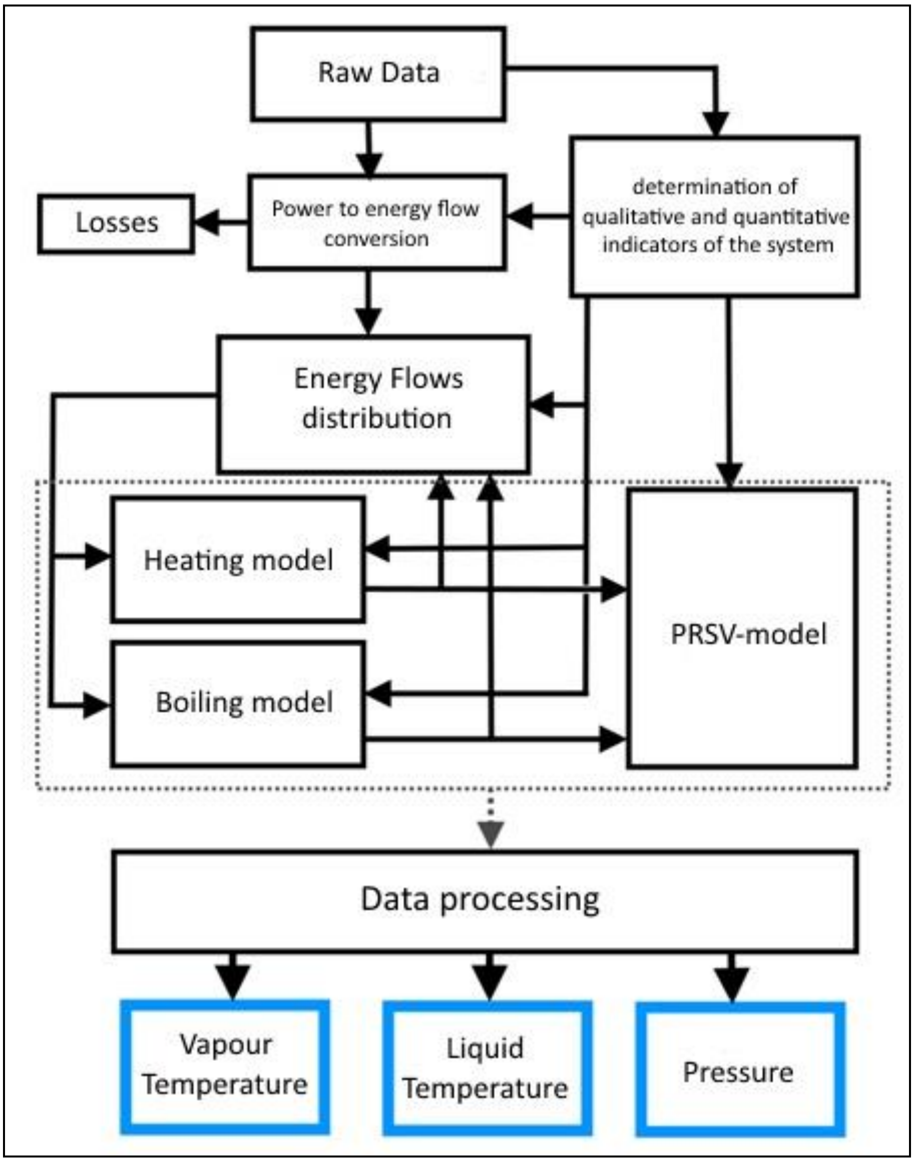

Figure 3. Mathematical model.

Schedules of verification of the data obtained from digital model are submitted in figures A1-A3. As it is possible to be convinced result of work of digital model corresponds to real data quite precisely, on average with small deviations to 5%.

Table 1. Results of quality of modeling.

	Liquid temperature	Vapour temperature	Pressure
Model error SKO	0,20	0,36	0,37
Correlation coefficient	0,87	0,79	0,83
The given model error	0,61	0,6	0,67
Average error of model	0,18	0,10	0,19

Deviations from real data generally appear for the account:

- Insufficient degree of accuracy of model;
- Errors of discrete blocks;
- Insufficient degree of study and popularity of some constants; for example, thermolysis coefficients;
- Lack of interrelations of model with external systems.

In general, as it is possible to be convinced, despite dot deviations, schedules correspond to experimental data quite precisely. Therefore, the created model corresponds to definition of the digital twin, and requirements imposed to them.

5. Conclusions

As a result of the done work, the main problems in the chemical industry have been analyzed today and also the existing ways of their decision have been established. As the main solved problem the problem of transition of the chemical industry to digital data has been chosen. As one of the technologies which are directly connected with the solution of this problem the technology of digital doubles is. Development of technology of creation of the last is the main objective pursued during this final qualification work.

First of all, for the solution of the chosen problem laboratory installation for division of binary aqueous-alcoholic mix for which cube part it was planned to create the digital twin has been chosen. In the beginning rectifying installation has been modified in a necessary way. In the picked-up, most important points of a column control sensors from which data, after the column run, through the operating Arduino payment, got to the computer where were processed in in advance prepared system created on the basis of the software of MatLab have been installed. The processed data remained further for verification of the model created in the future.

After has been launched installations and necessary data have been obtained, the market of the modern software for digital modeling has been analysed, and, after the analysis the modeling Simulink environment has been chosen.

Creation of mathematical model which included all fundamental laws and the principles of work of heating capacity was the following step after software choice. This mathematical model has been transferred further to Wednesday digital modeling of Simulink in which the digital double of the modelled object has been created. These works of the digital double have been verified according to work of the real column equipped with the heater. On the basis of the done work it is possible to draw the following conclusions:

1. By results of verification of results of work it is possible to tell that the accuracy of the created digital model is sufficient to be called the digital twin. Moreover, reaction of model to change of external factors very probably reflects reaction of real installation.

2. The environment of creation Matlab/Simulink is rather exact and convenient tool with extensive opportunities. Therefore, for creation of models in the future, this environment can be recommended for use.

3. The approach to creation of model used in work in general was quite rational and fast. The used equipment, and technology solutions attached to this equipment in general satisfy the accuracy of the digital twin.

Application A

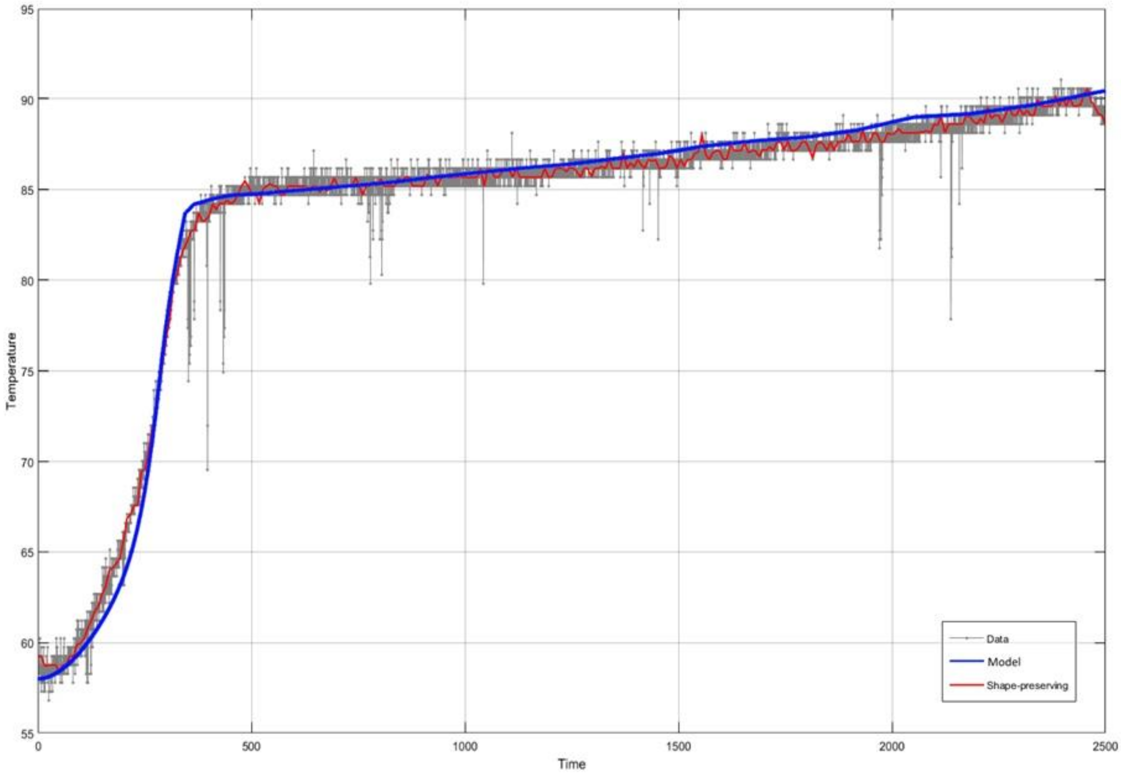

Figure A1. model verification results for cube fluid temperature.

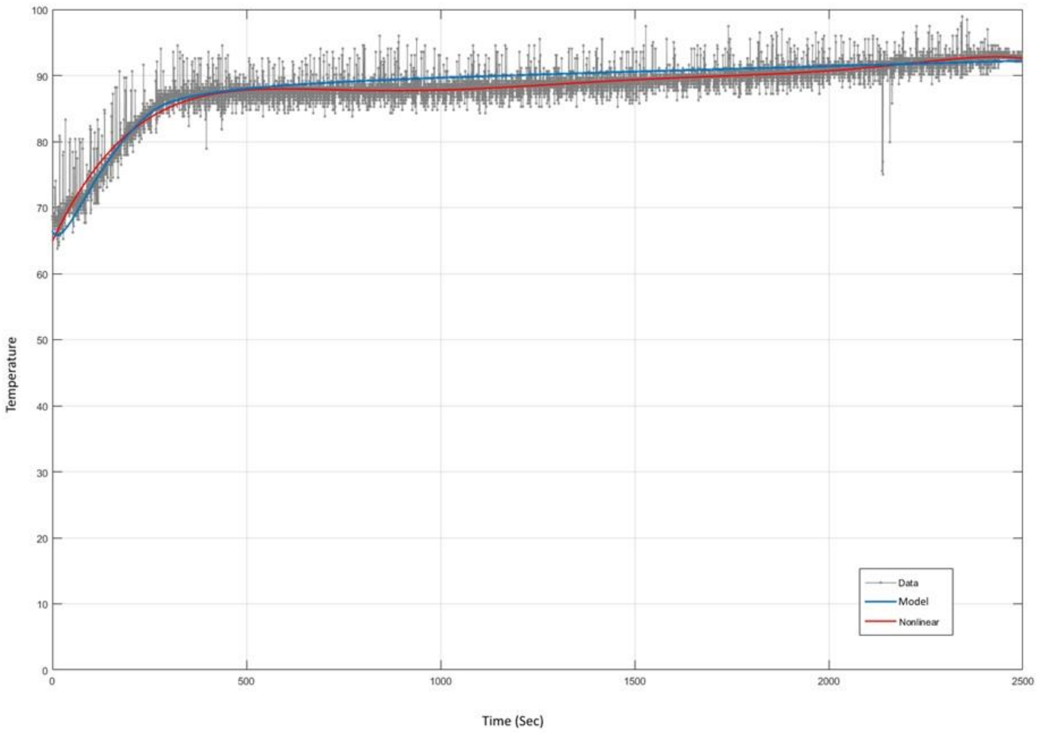

Figure A2. model verification results for cube gas temperature.

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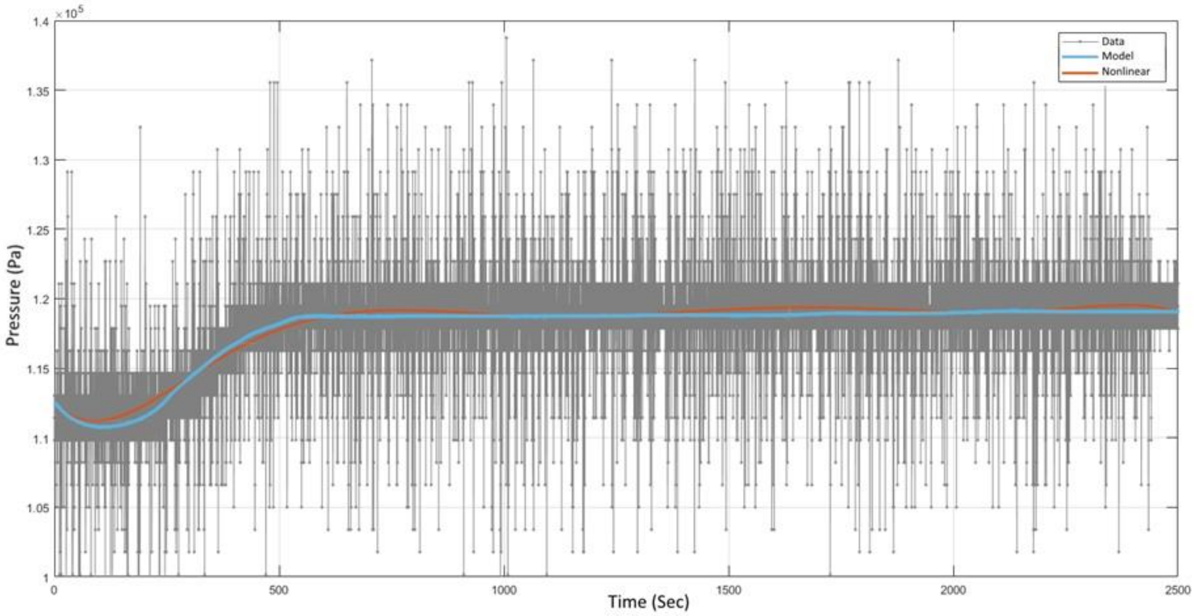

Figure A3. Pressure model verification results.

Application B

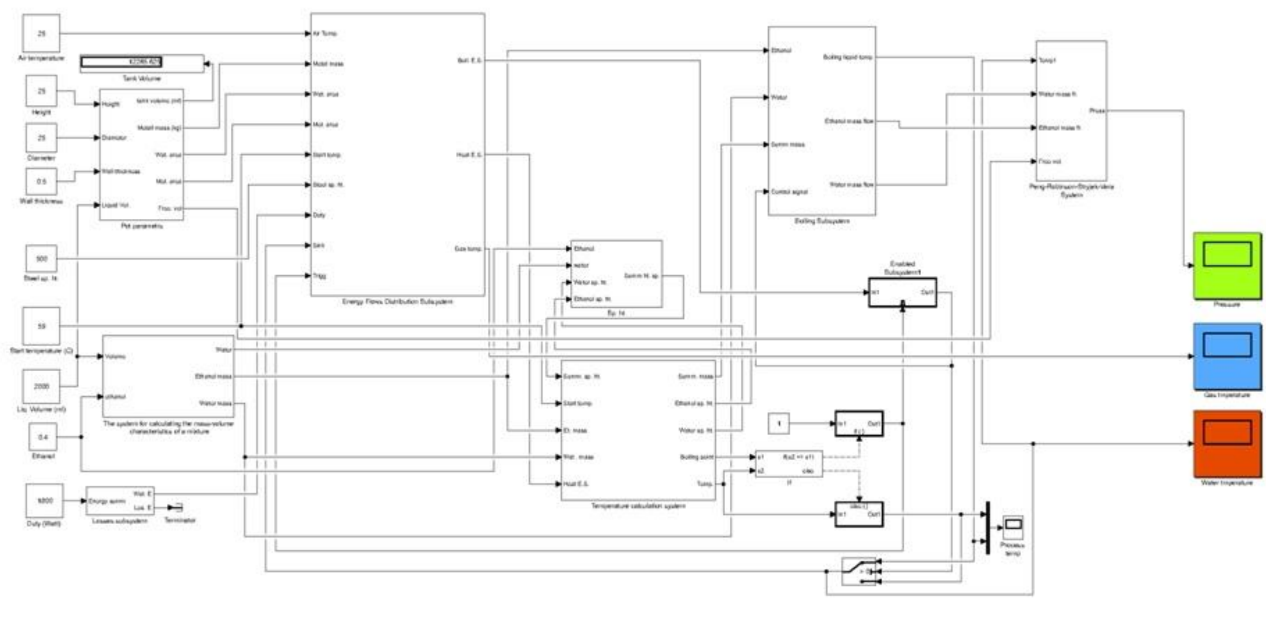

Figure B1. Simulink model.

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