Application of mathematical modelling in the process of design and production of pressure vessels

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Abstract. The paper presents the engineering practice, which the company ‘Regeneracija’ Ltd. Velika Kladuša – Bosnia and Herzegovina uses to perform preliminary experimental testing and measurements, followed by mathematical modeling of critical pressure of these vessels, in order to obtain the projected quality of pressure vessels made of composite materials. The paper will confirm the hypothesis that it is possible to relate mathematical connection and dependence of the critical pressure of vessels of composite materials (Pkr) with mechanical characteristics of vessel material (σM), vessel diameter (D), and vessel wall thickness (s). In this way, by varying the mentioned parameters, it is possible to achieve the desired product quality in the production of composite material containers by achieving the projected critical and thus working pressure. Generally speaking, the mathematical model of critical pressure obtained in this way will be a good indicator for design engineers to know how much critical pressure a given vessel can withstand, and based on that to take quick control of working or projected pressure, but also for designing completely new vessels made of composite materials as a substitute for the expensive experimental testing.

1. Introduction

Today's modern structures require new materials with special properties and shapes that can meet specific operating conditions: increased strength, resistance to pressure, temperature, speed, impact, vibration, etc. The purpose of new construction materials is to respond to increasingly complex requirements in terms of durability and the performance of modern constructions, as well as increasing restrictions on their weight. In order for the set requirements to be met, a compromise is inevitable in achieving light construction and high mechanical properties of the material. The application of composite materials enables the fulfillment of such set requirements [1].

One of the important parameters for engineers who deal with the design of pressure vessels made of composite materials is to know at what pressure the failure or cracking of the vessels will occur in relation to the selected combination of materials. The values of this critical pressure also depend on the orientation of the reinforcement in the composite. As it is known that a composite material consists of a matrix (polyester resin) and reinforcement (two types of reinforcement, mat and mat-rowing), it is difficult to define the characteristics of the material without experimental methods.

Designers face major problems when designing composite vessels, as there are many manufacturers of resin as well as glass reinforcements on the market, thus different combinations give different material characteristics. Pressure vessels made of composite materials are mainly used for water treatment such as sand filters, water softeners, active carbon filters, etc., as well as pressure...
vessels in air purification plants that are made in horizontal and vertical versions with a diameter of 500 (mm) to 2400 (mm), in classes 2, 4, 5, 6 and 10 (bar) [1].

In order to obtain the necessary results, i.e., the input parameters required for mathematical modeling, experimental tests were performed. The first part of the experiment referred to the definition of the mechanical characteristics of specimens made of composite materials, while the second part of the experiment referred to the definition of the critical pressure at which the vessels will yield. After obtaining the experimental results, mathematical modeling of the critical pressure will be performed based on the input-output parameters of the process. Thus, experimental measurements and mathematical modeling will prove that the critical pressure of composite materials can be related to the mechanical characteristics of the material (σM), diameter (D) and vessel wall thickness (s), i.e., that \( P_{kr} = f (s, D, \sigma_M, ...) \). In this way, by varying the mentioned parameters, it is possible to achieve the desired product quality in the production of vessels made of composite materials by achieving the projected critical and thus working pressure [1].

2. Analysis of the results of experimental testing

As already mentioned, different materials for making composites are offered on the market, so that when choosing different materials, it is possible to obtain different mechanical characteristics of the final composite. For these reasons, prior to making critical pressure test vessels, it is necessary to make composite tubes and test their mechanical properties. In the first experiment, tensile strength, modulus of elasticity and final elongation were obtained for two types of test tubes, and in the second experiment the values of critical pressures for eight tested vessels were obtained through previous research [2].

Table 1 shows the mean values of the obtained results, so that an increase in the mechanical properties of the material is seen when applying reinforcement in the form of rowing. Table 2 shows the results of experimental tests, i.e., the values of the measured achieved critical pressures for all eight tested vessels.

| Tube mark | Rupture force \( F_M \) (KN) | Tensile strength \( \sigma_M \) (MPa) | Modulus of Elasticity \( E \) (MPa) | Final elongation \( \varepsilon \) (%) |
|-----------|-----------------|-----------------|-----------------|-----------------|
| A         | 9.74            | 118.09          | 6591.86         | 2.70            |
| B         | 13.60           | 161.21          | 8177.09         | 2.56            |

Table 2. The results of measured critical pressure [2].

| No | D (mm) | s (mm) | \( \sigma_M \) (N/mm²) | Experimental results \( P_{kr} \) (bar) |
|----|--------|--------|------------------------|-------------------------------------|
| 1  | 400    | 3.2    | 118                    | 22.0                                |
| 2  | 800    | 3.2    | 118                    | 9.0                                 |
| 3  | 400    | 6.4    | 118                    | 30.0                                |
| 4  | 800    | 6.4    | 118                    | 17.0                                |
| 5  | 400    | 3.2    | 161                    | 26.5                                |
| 6  | 800    | 3.2    | 161                    | 12.5                                |
| 7  | 400    | 6.4    | 161                    | 35.0                                |
| 8  | 800    | 6.4    | 161                    | 20.5                                |

The previous table shows the obtained results of critical pressure \( (P_{kr}) \) measurements for eight experimentally tested vessels depending on the diameter (D), wall thickness (s) and material characteristics \( (\sigma_M) \).
It should be emphasized that in the first four vessels, which were made with mat reinforcements, there was total damage during cracking, as shown in figure 1.a). Due to the action of circular stress, the cylindrical part of the vessel yielded, causing a crack along the entire vessel, i.e. along the cylindrical part of the vessel [2].

![Figure 1. a) Shape of yielding of vessels made of mat reinforcement (left)
    b) Shape of yielding of vessels made of mat and rowing reinforcement (right).](image)

The other four vessels, which have continuous rowing in their structure, yielded only in one place at the moment of critical pressure, as shown in figure 1.b). Due to the yielding of the vessel under a certain pressure, continuous fibers did not allow the crack to be transferred to the rest of the vessel but localized the crack, which gives vessels that have rowing in their structure a huge advantage for safety reasons [2].

According to table 2, it can be seen that increasing the diameter of the vessel decreases the value of the critical pressure, while the increasing the wall thickness increases its value. The table also shows the influence of the mechanical properties of the materials, i.e., the value of the critical pressure grows with their increase.

### 3. Mathematical modelling of critical pressure

Experimental tests are used to check, correct and verify numerical results, and mathematical modeling that most realistically describes machining processes and systems. Technological design and engineering of modern machining processes require the analysis of all technical and technological parameters of the process and the application of scientific methods in order to model and define the optimum conditions of processing systems and processes [3].

In this paper, it is necessary to obtain a mathematical model for critical pressure based on the input parameters and the results of experimental tests. The goal is to define the final critical pressure to which the vessel can withstand the load, i.e., pressure, by changing the input parameters.
3.1. Selection of influential process or system parameters

In order to perform an experiment, it is necessary to limit it beforehand, i.e., it is necessary to isolate several influencing factors from a large number of them, as well as the output value to be measured. Since the task in this paper is to obtain a mathematical model for critical pressure, figure 2 shows the parameters that will be selected to influence this process.

Figure 2. Scheme of input - output parameters [2].

Which are as follows:

TO  ambient temperature;
VO  ambient humidity;
HUO  chemical impact of the environment.

These influential factors, as independent variables, are called the basic factors that vary during the performance of the experiment according to predetermined limits and the plan of the experiment. Other influential factors, whose influence is neglected or kept unchanged during the experiment, are called external factors [3].

The basic factors are selected so that their changes are not functions of external factors nor are they interrelated and it is relatively possible to perform their measurement in the process. The factors were varied within the limits shown in table 4.

Table 3. Variables and experiment results.

| No. | X₁ (D (mm)) | X₂ (s (mm)) | X₃ (σ₀(N/mm²)) | Pₚₐ (bar) |
|-----|-------------|-------------|-----------------|-----------|
| 1   | 400         | 3.2         | 118             | 22.0      |
| 2   | 800         | 3.2         | 118             | 9.0       |
| 3   | 400         | 6.4         | 118             | 30.0      |
| 4   | 800         | 6.4         | 118             | 17.0      |
| 5   | 400         | 3.2         | 161             | 2.5       |
| 6   | 800         | 3.2         | 161             | 12.5      |
| 7   | 400         | 6.4         | 161             | 35.0      |
| 8   | 800         | 6.4         | 161             | 20.5      |
Table 4. Influencing experiment factors.

| EXPERIMENT LEVEL | Influencing factors |
|------------------|--------------------|
|                  | D (mm) | s (mm) | $\sigma_M$ (N/mm$^2$) |
| Minimum          | 400    | 3.2    | 118               |
| Maximum          | 800    | 6.4    | 161               |

In order to create a plan of the experiment matrix, it is necessary to encode the basic factors, and transport them into the space of coded coordinates. The factor variation interval represents half of the difference between the largest ($x_{i\text{ max}}$) and smallest ($x_{i\text{ min}}$) values of the $i$-th parameter ($i = 1, 2, 3$), and can be defined as follows:

$$\Delta x_i = \frac{x_{i\text{ max}} - x_{i\text{ min}}}{2}$$

(1)

The interval of variation of the $i$-th factor should be chosen so that it adequately represents the basic factor in the examined area. Coded values are always used in the paper because it makes it easier to calculate and form the plan of the experiment matrix. The coding is performed as follows:

$$X_i = \frac{x_i - x_{0i}}{\Delta x_i} = \frac{x_i - x_{0i}}{\frac{x_{i\text{ max}} - x_{i\text{ min}}}{2}}$$

(2)

Explained as:

- $X_i$ coded value of independent variables
- $i$ number of independent variables ($i = 1, 2, 3, ...$)
- $x_i$ physical value of independent variables at the upper or lower level
- $x_{0i}$ physical value of independent variables in the center of the plan, i.e., zero mean value
- $\Delta x_i$ interval of the limit of physical values of variables from the midpoint to the maximum, i.e., minimum values of the variable

The average level of physical value is determined by the expression:

$$x_{0i} = \frac{x_{i\text{ max}} + x_{i\text{ min}}}{2}$$

(3)

The coded values, as can be seen, are dimensionless quantities. Coding transfers the coded origin to the zero point of the experiment, as the central point of the experiment (which corresponds to the mean level of all three factors). Coding for the $i$-th factor is as follows:

$$X_i = +1 \quad \text{for factor } x_i = x_{i\text{ max}}$$
$$X_i = -1 \quad \text{for factor } x_i = x_{i\text{ min}}$$

3.2. Selection of influential process or system parameters

When selecting the type of mathematical model, there is no generally valid rule. This means that for each researched process or system, a model should be chosen and its accuracy and adequacy in relation to the actual real process should be checked. In this experiment, three independent variables were selected, and thus there are three variable factors, i.e., $k = 3$, while the variation of the factor is at two levels $r = 2$ (min and max), which means that it has the character of a three-factor experiment plan where needed number of measurements is:

$$N = r^k = 2^3 = 8$$

(4)
number of levels of basic factors \((r = 2, \text{min and max})\)

number of varied basic factors \((k = 3)\)

number of repetitions of the experiment with factor variation \((N=8)\)

The initial mathematical model is a first-order three-factor polynomial:

\[
Y = b_0 + b_1 X_1 + b_2 X_2 + b_3 X_3
\]

Table 5. Experiment plan matrix.

| No. | \(X_0\) | \(X_1\) | \(X_2\) | \(X_3\) | \(y_j\) |
|-----|---------|---------|---------|---------|--------|
| 1   | 1       | -1      | -1      | -1      | 22.0   |
| 2   | 1       | 1       | -1      | -1      | 9.0    |
| 3   | 1       | -1      | 1       | -1      | 30.0   |
| 4   | 1       | 1       | 1       | -1      | 17.0   |
| 5   | 1       | -1      | -1      | 1       | 26.5   |
| 6   | 1       | 1       | -1      | 1       | 12.5   |
| 7   | 1       | -1      | 1       | 1       | 35.0   |
| 8   | 1       | 1       | 1       | 1       | 20.5   |

Coefficients of mathematical model:

\[
b_0 = \frac{1}{N} \sum_{j=1}^{N} X_{ij} y_j \quad \text{for...} i = 1, 2, 3, \ldots, k
\]

\[
b_i = \frac{1}{N} \sum_{j=1}^{N} X_{ij} y_j \quad \text{for...} 1 \leq i < m \leq k
\]

Expedented as:

\(X_{ij}\) value of \(X_i\) in j-th experiment

\(y_j\) measured size in j-th experiment

number of experiments

\[
b_0 = \frac{1}{8} (y_1 + y_2 + y_3 + y_4 + y_5 + y_6 + y_7 + y_8)
\]

\[
b_1 = \frac{1}{8} (-y_1 + y_2 + y_3 - y_4 + y_5 + y_6 - y_7 + y_8)
\]

\[
b_2 = \frac{1}{8} (-y_1 - y_2 + y_3 + y_4 - y_5 + y_6 - y_7 + y_8)
\]

\[
b_3 = \frac{1}{8} (-y_1 - y_2 - y_3 - y_4 + y_5 + y_6 + y_7 + y_8)
\]

Table 6. Model coefficients.

| \(b_0\) | 21.5625 |
| \(b_1\) | -6.8125 |
| \(b_2\) |  4.0625 |
| \(b_3\) |  2.0625 |

By including the coefficients from the previous table in the form (5), the following is obtained:

\[
Y = 21.56 - 6.81X_1 + 4.06X_2 + 2.06X_3
\]
3.3. Selection of influential process or system parameters

To assess the adequacy of the model, i.e., to examine the relationship between the dependent variable quantity \( y_j \) and the independent variable quantity \( X_i \), the multiple regression coefficient is used as follows:

\[
R = \sqrt{1 - \frac{\sum_{j=1}^{N} (y_j^E - \bar{y}_j)^2}{\sum_{j=1}^{N} (y_j^E - \bar{y}_j)^2}}
\]  

(10)

Explained as:

- \( y_j^E \) values of experimental results
- \( y_j^R \) calculated values from the obtained model
- \( \bar{y}_j \) arithmetic mean of all experimental results

| No | \( y_j^E \) | \( y_j^R \) | \((y_j^E - y_j^R)^2\) | \((y_j^E - \bar{y}_j)^2\) |
|----|-----------|-----------|----------------|----------------|
| 1  | 22.0      | 22.3      | 0.090          | 0.19           |
| 2  | 9.0       | 8.7       | 0.090          | 157.75         |
| 3  | 30.0      | 30.4      | 0.160          | 71.23          |
| 4  | 17.0      | 16.8      | 0.040          | 20.79          |
| 5  | 26.5      | 26.4      | 0.010          | 24.40          |
| 6  | 12.5      | 12.8      | 0.090          | 82.08          |
| 7  | 35.0      | 34.5      | 0.250          | 180.63         |
| 8  | 20.5      | 20.9      | 0.160          | 1.12           |

\[ \bar{y}_j = 21.56 \]
\[ \Sigma = 0.89 \]
\[ \Sigma = 538.19 \]

The values of the multiple regression coefficients are in the range \( 0 \leq R \leq 1 \). When the value of the coefficient is \( R=1 \), the model fully describes the results of the experiment. The value \( R=0 \) shows that there is no interdependence between the variables \( y_j \) and \( X_i \) [3].

By including the obtained values in expression (10), the coefficient of multiple regression \( R=0.999 \) is obtained. The obtained value of the multiple regression coefficient indicates that the mathematical model (9) adequately describes the mentioned process, i.e., with 99.9%.

Decoding:

\[
X_1 = \frac{D - D_{min} + D_{max}}{2} = \frac{D - \frac{800+400}{2}}{800-400} = \frac{D - 600}{200}
\]

\[ X_1 = (0.005D - 3) \]  

(11)

\[
X_2 = \frac{s - s_{min} + s_{max}}{2} = \frac{s - \frac{6.4 + 3.2}{2}}{6.4 - 3.2} = \frac{s - 4.8}{1.6}
\]

\[ X_2 = (0.625s - 3) \]  

(12)

\[
X_3 = \frac{\sigma_M - \sigma_{M_{max}} + \sigma_{M_{min}}}{2} = \frac{\sigma_M - \frac{161+118}{2}}{161 - 118} = \frac{\sigma_M - 139.5}{21.5}
\]

\[ X_3 = (0.0465\sigma_M - 6.488) \]  

(13)
By including the decoded values, the final mathematical form is obtained:

\[ P_{kr} = 21.56 - 6.81(0.005D - 3) + 4.06(0.625s - 3) + 2.06(0.0465\sigma_m - 6.488) \]  \hspace{1cm} (14)

That is:

\[ P_{kr} = 16.445 - 0.034D + 2.538s + 0.096\sigma_m \]  \hspace{1cm} (15)

The dependence of the critical pressure \((P_{kr})\) on the input parameters (vessel diameter - \(D\), wall thickness - \(s\), and material characteristics - \(\sigma_m\)) can be shown in the diagram, as shown in the following figure.

![Figure 3. Dependence of critical pressure and tensile strength [4].](image)

As an illustrative example, Figure 3 shows the dependence of the critical pressure and tensile strength of the material, with constant values of the diameter and wall thickness of the vessel.

3.4. Selection of influential process or system parameters
The obtained mathematical model of critical pressure (15) is a good indicator for designers to know which critical pressure the vessel can withstand, and base on that to make a quick control of the working or projected pressure.

The presented mathematical model for the tested pressure vessels gives results with a deviation of \(\pm 0.5\) (bar) in relation to the experimental results, so that it can be said with accuracy at which pressure the total damage to the vessel will occur, i.e., failure or cracking of pressure vessels.

Table 8 shows the comparative results obtained according to mathematical modeling and according to experimental measurements.
Table 8. Results of critical pressure of experiment and mathematical model.

| N  | X₁ (D mm) | X₂ (s mm) | X₃ (σₓₓ(N/mm²)) | Pkr exp (bar) | Pkr mat (bar) |
|----|-----------|-----------|-----------------|---------------|--------------|
| 1  | 400       | 3.2       | 118             | 22.0          | 22.1         |
| 2  | 800       | 3.2       | 118             | 9.0           | 8.5          |
| 3  | 400       | 6.4       | 118             | 30.0          | 30.3         |
| 4  | 800       | 6.4       | 118             | 17.0          | 16.7         |
| 5  | 400       | 3.2       | 161             | 26.5          | 26.3         |
| 6  | 800       | 3.2       | 161             | 12.5          | 12.7         |
| 7  | 400       | 6.4       | 161             | 35.0          | 34.4         |
| 8  | 800       | 6.4       | 161             | 20.5          | 20.8         |

The results of the mathematical model shown in table 8 for the tested pressure vessels show deviation of ±0.5 (bar) in relation to the experimental results, so that it can be known with great accuracy at which pressure the vessel will be completely damaged, i.e., the vessel will crack.

4. Recommendations for designers and production technologists

The European standard EN 13923 determines the material, design and testing of pressure vessels made of composite materials.

Design factor:
Permissible stress in each layer of load-bearing laminate is derived from characteristic elasticity and strength, material safety factor S, inhomogeneity (A₁), chemical influence (A₂), design temperature in relation to heat resistance (A₃), dynamic load effect (A₄) and long-term behavior (A₅).

The design factor is calculated according to the form:

\[ K = S \cdot A₁ \cdot A₂ \cdot A₃ \cdot A₄ \cdot A₅ \]  \hspace{1cm} (16)

The safety factor S must be a minimum of 2, while the partial factors A₁ to A₅ are given in table 9. It should be emphasized that the total value of the design factor (K) must not be less than 4.

Table 9. Partial design factors.

| Partial design factors | Min. value | Max. value |
|------------------------|------------|------------|
| A₁                     | 1.00       | 2.00       |
| A₂                     | 1.10       | 1.80       |
| A₃                     | 1.00       | 1.40       |
| A₄                     | 1.00       | 1.10       |
| A₅                     | 1.25       | 2.00       |

Maximum allowed dilatation:
The maximum allowable dilatation is calculated on the basis of the limited dilatation \( \varepsilon_{\text{lim}} \) and the partial factor of long-term behavior A₅.

\[ \varepsilon_{\text{max}} = \frac{\varepsilon_{\text{lim}}}{A₅} \]  \hspace{1cm} (17)
According to standard EN 13121-2, the dilatation must not exceed 0.25 % for all types of protective layer. Table 10 shows the limiting dilatation for three types of resins reinforced with spray rowing or with mat 900 (g/m²).

**Table 10. Limiting dilatation of the protective layer.**

| Type of resin                        | $\varepsilon_{\text{lim}}$          |
|--------------------------------------|-------------------------------------|
| UP (unsaturated polyester resin)     | $\min (0.1 \times \varepsilon_{\text{resin}} \, \text{ili} \, 0.20\%)$ |
| VE (vinyl ester resin)               | $\min (0.1 \times \varepsilon_{\text{resin}} \, \text{ili} \, 0.25\%)$ |
| EP (epoxy resin)                    | $\min (0.1 \times \varepsilon_{\text{resin}} \, \text{ili} \, 0.30\%)$ |

$\varepsilon_{\text{resin}}$ - resin dilatation

Conditions of loads and dilatations:

Loads and dilatations must meet the following conditions:

$$\sigma_c = \frac{DP}{2s} \leq \frac{\sigma_M}{K}$$  \hspace{1cm} (18)

$$\sigma_m = \frac{DP}{4s} \leq \frac{\sigma_M}{K}$$  \hspace{1cm} (19)

$$\varepsilon_c = \frac{\sigma_c}{E_c} \leq \varepsilon_{\text{max}}$$  \hspace{1cm} (20)

$$\varepsilon_m = \frac{\sigma_m}{E_m} \leq \varepsilon_{\text{max}}$$  \hspace{1cm} (21)

Explained as:

- $\sigma_c$ circular load
- $\sigma_m$ meridian load
- $P$ pressure in the vessel
- $\sigma_M$ yield strength, in which case there are two types of materials:
  - yield strength of mat composites, $\sigma_M = 118 \, \text{N/mm}^2$
  - yield strength of composites with mat and rowing, $\sigma_M = 167 \, \text{N/mm}^2$
- $E_c$ circular modulus of elasticity, in which case there are two types of materials:
  - modulus of elasticity of mat composites, $E = 6592 \, \text{N/mm}^2$
  - modulus of elasticity of composites with mat and rowing, $E = 8177 \, \text{N/mm}^2$
- $E_m$ meridian modulus of elasticity (moduli of elasticity in circular and meridian directions are equal)
- $\varepsilon_c$ circular dilatation
- $\varepsilon_m$ meridian dilatation

Table 11 shows the obtained working pressures that were reached on the basis of the conditions shown in the previous expressions.
Table 11. Working pressures of vessels tested to critical pressure.

| N | Vessel diameter D (mm) | Wall thickness s (mm) | Tensile strength $\sigma_m$ (N/mm$^2$) | Operating pressure $P_{rad}$ (bar) |
|---|------------------------|-----------------------|--------------------------------------|----------------------------------|
| 1 | 400                    | 3.2                   | 118                                  | 4.72                             |
| 2 | 800                    | 3.2                   | 118                                  | 2.36                             |
| 3 | 400                    | 6.4                   | 118                                  | 9.44                             |
| 4 | 800                    | 6.4                   | 118                                  | 4.72                             |
| 5 | 400                    | 3.2                   | 161                                  | 6.44                             |
| 6 | 800                    | 3.2                   | 161                                  | 3.22                             |
| 7 | 400                    | 6.4                   | 161                                  | 12.88                            |
| 8 | 800                    | 6.4                   | 161                                  | 6.44                             |

Considering that there are various combinations of composite materials on the market, in order to be able to design the working pressure, the best option is to conduct experimental research, and based on that perform mathematical modeling of critical pressure, i.e., working pressure, as shown in this paper.

5. Conclusion
The research results in this paper have shown that experimental research and measurements can lead to very useful results that can serve as input data for the development of a mathematical model of the critical pressure of pressure vessels made of composite materials.

The development of a mathematical model confirmed the hypothesis that it is possible to bring into a mathematical relationship and dependence the critical pressure of vessels made of composite materials with mechanical characteristics of composite material of vessel ($\sigma_m$), vessel diameter (D) and vessel wall thickness (s). The obtained mathematical model for the tested pressure vessels gives results with a deviation of $\pm 0.5$ (bar) in relation to the experimental results, so that it can be determined with good accuracy at which pressure the vessel will fail or crack.

The mathematical model of critical pressure obtained in this way is a good indicator for designers to know how much critical pressure the specified vessel can withstand, based on which they can make a quick control of the working or projected pressure. In this way, by varying the mentioned parameters, it is possible to achieve the desired product quality by achieving the projected critical and thus working pressure in the production of pressure vessels made of composite materials.

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