# Research on the Flow Law and Mechanical Properties of Polymers Based on Finite Element Analysis

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**Abstract:Polymer grouting technology has demonstrated significant advantages in maintenance and repair projects and has been widely applied in various fields such as road repair, building rectification, foundation reinforcement, mechanical structure enhancement, and leakage prevention and repair. Based on the analysis of domestic and international research on polymer grouting technology and application cases, this paper studies the fluidity and diffusion mode of polymer materials, and also explores their mechanical properties. The research shows that the fluidity and reactivity of polymer grouting materials are strongly influenced by temperature and time; as the temperature rises, the chemical reaction rate increases, because high temperatures accelerate the chemical reaction process, causing the grout to solidify faster, indicating a positive influence of temperature and time on viscosity. Additionally, polymer materials possess excellent compressive, tensile, and shear resistance capabilities, and their performance can be effectively applied in engineering fields that require bearing significant loads. This paper investigates the flow patterns and mechanical properties of polymers, and the experimental data obtained provide examples for related fields, facilitating the research of new technologies and processes for polymer materials**

**Keywords: Mechanical Properties of Polymers; Polymer Grouting; Polymer Materials; Chemical Reaction**

## 1. Introduction

The maintenance and upkeep requirements from China's massive infrastructure and mechanical equipment are very severe, requiring a large amount of manpower and financial resources every year. Polymers have been widely used in road repair[1-3]. Domestic maintenance technology still mainly relies on traditional maintenance methods, which have many shortcomings. A high polymer is a macromolecular compound composed of many molecules bonded by covalent bonds. It is not only light in weight, high in toughness and high in strength[4], it has high physical and chemical properties and operational space, and can be used in many fields[5]. Polymer grouting technology is a more efficient and better maintenance quality technology, which mainly uses polymer materials injected into the foundation structure to play a maintenance role. Compared with traditional maintenance methods, high polymer grouting technology has advantages such as fast solidification speed, high grouting material strength, low density, and strong adaptability.It facilitates chemical recycling[6]. It can be used to fix hidden defects[7].

Polyurethane adhesive was used to bond metal and butadiene rubber to tank tracks as early as World War II and Polyurethane is also used in coatings because it enhances the life of the metal. It is used to shield against electromagnetic interference[8] and enhance dielectric.In 1947, DuPont Monsanto started to manufacture rigid polyurethane foam. In 1974, Americans used the polyurethane RIM process to produce car fenders and car body. Since 1989, polymer grouting technology has been applied in over 75000 projects worldwide, solving a large number of engineering problems . Today, polymer grouting technology has been promoted and applied in more than 50 countries, including China . At present, this technology is widely used for the reinforcement, maintenance, additive manufacturing[9] and repair of infrastructure such as roads, bridges, tunnels, buildings, heat insulation[10]and sound absorption[11] .The radiation non-projectivity of polyurethane is also widely used in the medical field[12] and its process flow is gradually optimized in practice. Its performance can be affected by factors such as ambient temperature, humidity, and external loads[13]. Therefore, research should focus on the key components and reaction steps in the raw material system, and extract key parameters for numerical simulation to ensure the accuracy and practicality of the model. Polyurethane is selected as the type of polymer for study in this article.

## 2. Principles of Polymer Chemical Reactions

Polyurethane is produced by the reaction of isocyanates, polyols, catalysts, water, and other necessary substances.(The reaction of isocyanates, polyols, catalysts, water, and other necessary substances produces Polyurethane.) When the raw materials are mixed, the chemical reaction immediately begins. After about 40 to 60 seconds of mixing, the density of the polyurethane mixture begins to significantly decrease. The entire reaction process is highly exothermic[14], with the temperature at the center of the mixture reaching up to 150 ° C or higher. The filling process is mainly divided into two simultaneous reactions - gel reaction and foaming reaction.

### 2.1 Gel Reaction

The gel reaction of polyurethane refers to the gel phenomenon during the reaction of isocyanate and polyol to form polyurethane during the preparation of polyurethane. Its chemical reaction equation (1.1) is shown in the the following figure[15].

$$2\mathrm{R{-}NCO+H_2O \rightarrow RNHCOOR'+CO_2} \qquad (1)$$

### 2.2 Foaming Reaction

The foaming reaction of polyurethane involves the reaction between isocyanates and water in material A. The chemical equation for foaming reaction is:

$$R-NCO+H_2O \rightarrow R-NH_2+CO_2 \xrightarrow{R-NCO} RNHCOOR' \qquad (2)$$

According to S A. The simplified model proposed by Baser (1994) simplifies the entire chemical reaction as follows:

$$2R-NCO+H_2O \rightarrow RNHCOOR'+CO_2 \qquad (3)$$

The physical properties of high polymer polyurethane are influenced by its specific formula, structure, and preparation method, so there may be a certain range of variation. The general description is as follows:

**Table 1. Polyurethane Material Properties**

| Material properties | Attribute value |
|---|---|
| density | 1100kg/m3 |
| viscosity | 1.72e-05Pa·s |
| Thermal conductivity | 0.0454W/m·K |
| Specific heat capacity | 1800J/g·K |
| Molecular weight | 44kg/kmol |

The complete reaction process of polyurethane includes the gelation phenomenon and foaming reaction. In order to fully describe the filling process of polyurethane foam, the following assumptions are made.

(1). Suppose the foam is a homogeneous fluid.

(2). Assume that the mixture is well mixed.

(3). Ignore the inhomogeneity caused by incomplete mixing.

(4). Since the mixture has little change in volume and heat generation during the reaction, the gel reaction can be ignored during the simulation, and the foaming reaction is mainly studied.According to the literature reference, the properties of each material can be obtained asfollows:

## 3. Example of Polymer

Therefore, it can be determined by this experiment that the temperature is 25°Cand the grouting amount is 20ml as the control group, and the specific test parameter combination scheme is shown in Table 3.

**Table 3. Test Parameter Combination Table**

| Experiment number | Temperature°C | Injection volume ml |
|---|---|---|
| 1 | 25 | 20 |
| 2 | 35 | 20 |
| 3 | 45 | 20 |
| 4 | 25 | 15 |

**Table 2. FLUENT Setting Properties of Each Material**

| Material name | Density kg/m$^3$ | Viscosity Pa·s | Thermal conductivity W/m·K | Specific heat capacity J/g·K | Molecular weight kg/kmol |
|---|---|---|---|---|---|
| Carbon dioxide | 1.7878 | 1.37e-05 | 0.0145 | 840.37 | 44 |

| | | | | | |
|---|---|---|---|---|---|
| air | 1.225 | 1.7894e-05 | 0.0242 | 1006.43 | 28.966 |
| water | 998.2 | 0.001003 | 0.6 | 4182 | 18.0152 |
| isocyanates | 1080 | 5 | 0.015 | 200 | 144.1734 |

### 3.1 Experimental Results

Figure 1 below shows the reaction degree of polymers at different ambient temperatures under the same grouting amount conditions.

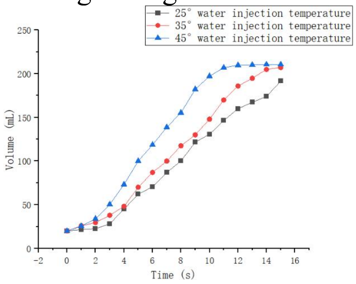
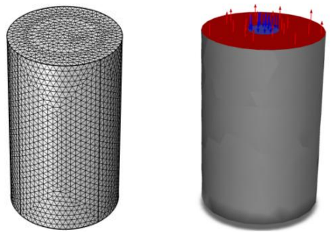


**Figure 1. The Degree of Reaction at Different Water Injection Temperatures**

It can be clearly seen from the volume change trend in Figure 2-6 that the higher the water injection temperature, the faster the reaction speed, from 0 seconds to 3 seconds is roughly the gel reaction stage, and the subsequent time is the foaming reaction stage. This is because in the gel reaction and foaming reaction to generate polyurethane, the temperature can significantly accelerate the molecular reaction rate, thereby accelerating the gel formation rate and the foam expansion rate.

### 3.2 Establishment of 3D Flow Field Simulation Model

As shown in Figure 2, construct a D=20 ~mm, h=30mm cylinder, the grid cell size is set to 0.4mm, select the central part of the top region of the cylinder as the inlet (inlet), the injected material will enter from this region, the size of the region is a circle with a radius of 1.5mm, the rest of the top region is the outlet (outlet), the internal material will flow out from this region, the size of the region is an outer diameter of 10mm, an inner diameter of 1.5mm annular, and the side and bottom surfaces of the cylinder are set as wall:



**(a) Grid Model (b) Force Application**

**Figure 2. Model Boundary Condition Settings**

### 3.3 Factors Affecting the Flow Characteristics of Polymers

Set up a single-factor controlled experiment to explore the effects of isocyanate capacity, temperature field, and water injection speed on the flow characteristics of polyurethane. Set up a set of control groups and three sets of variable groups. In order to analyze the data more intuitively, the middle section of the cylindrical surface is selected as the cloud map, and the center of the model is selected as the reference point, which is located at a height of 15mm in the cylindrical model. The mass fraction changes of isocyanate (r-nco) and polyurethane (r2n2h2co) at this point are studied to obtain the flow characteristics of the polymer.Moreover, in order to analyze the data more intuitively, the middle section of the cylindrical surface was selected as the cloud map, and the center of the model was chosen as the reference point, which is located at a height of 15mm in the cylindrical model. The mass fraction changes of isocyanate (r-nco) and polyurethane (r2n2h2co) at this point were studied to obtain the flow characteristics of the polymer. Figures 3 and 4 show the mass distribution of isocyanates in the control group and the mass fractions of isocyanates and polyurethanes at the reference point.

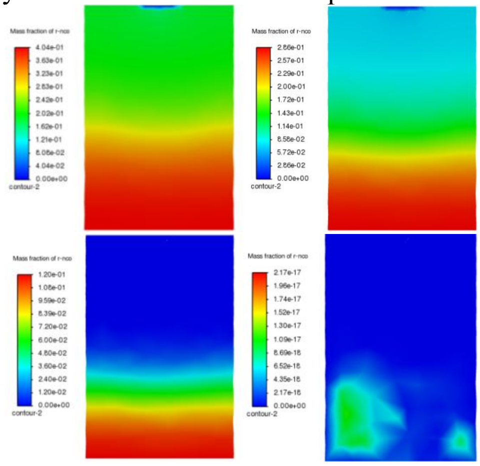


**Figure 3. Isocyanate Volume Fraction Cloud Maps at 2s, 4s, 6s, and 8s**

### 3.4 Influence of Isocyanate Volume

In order to investigate the effect of the initial volume of isocyanates on the reaction of polyurethane formation, parameters such as temperature field and water injection rate were kept constant, and only the volume of isocyanates was changed. The unit area of isocyanates was changed to a bottom radius of 10mm and a height of 4mm, placed at the bottom of the cylindrical model. The mass distribution of isocyanates and the mass fraction of isocyanates and polyurethane at the reference point are shown in Figures 5 and 6.

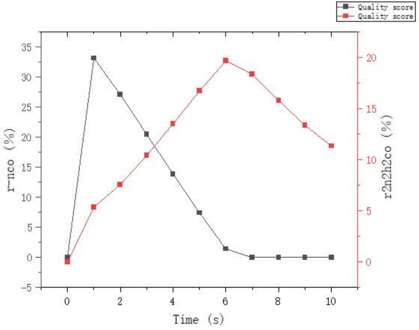


Figure 4. Changes in Mass Fractions of Isocyanates and Polyurethanes at Reference Points

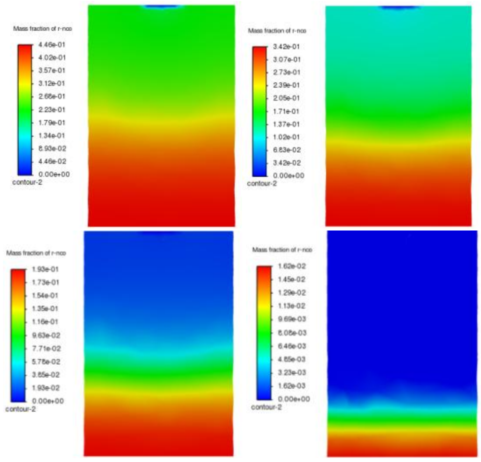


Figure 5. Isocyanate Volume Fraction Cloud Maps at 2s, 4s, 6s, and 8s

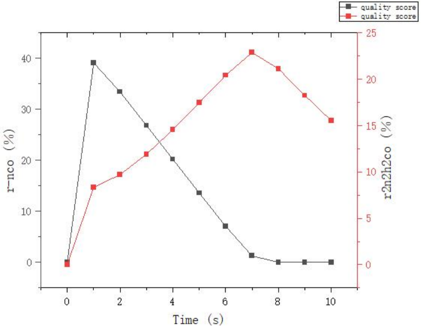


Figure 6. Changes in Mass Fractions of Isocyanates and Polyurethanes at Reference Points

When the volume of isocyanates increases, it can be clearly seen from Figure 5 that the isocyanates react completely in the 7th second, while the isocyanates in the control group react completely in the 6th second. Therefore, an increase in the volume of isocyanates can significantly increase the total reaction time.

When the water injection rate increases, it can be clearly seen from the above data that the isocyanate in the control group reacts completely in the 6th second, while in the table with a water injection rate of 0.1m/s, the reaction is complete in the 5th second. Therefore, an increase in the volume of isocyanate can significantly increase the total reaction time. Moreover, the maximum mass fraction of generated polyurethane is approximately 6% lower than that of the control group. This is because during the simulation process, an increase in water injection rate will result in more water occupying the space inside the container. Therefore, polyurethane with a faster injection rate will have a lower maximum mass fraction.

Figures 6 show the mass distribution of isocyanates and the mass fractions of isocyanates and polyurethane at the reference point when the injection rate of water is 0.2m/s.

When the water injection rate increases, it can be clearly seen from the above data that the isocyanate in the control group reacts completely in the 6th second, while in the table with a water injection rate of 0.2m/s, the reaction is complete in the 4th second. As a result, an increase in the volume of isocyanates can significantly increase the total reaction time.

Moreover, the maximum mass fraction of generated polyurethane is approximately 7% lower than that of the control group. This is also because during the simulation process, an increase in water injection rate will result in more water occupying the space inside the container. Therefore, a faster injection rate of polyurethane will have a lower maximum mass fraction.

### 3.5 Temperature Field Influence

Set the isocyanate volume to a bottom radius of 10 mm and a height of 3mm, place it at the bottom of a cylindrical model, with a water injection hole radius of 2.5mm and a water injection rate of 0.05m/s, and only change the size of the temperature field to study the effect of temperature field on the flow characteristics of the generated polyurethane, , it can be clearly seen from Figure 7 and Figure 8.

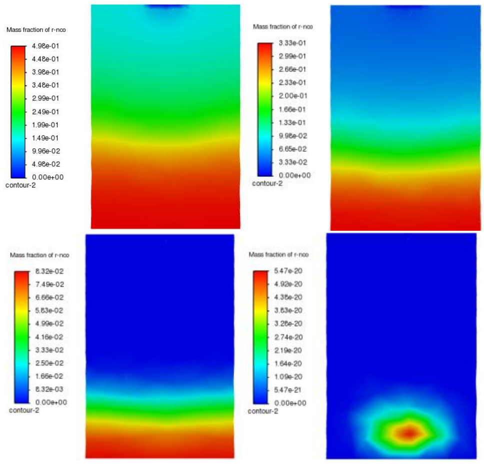


**Figure 7. Isocyanate Volume Fraction Cloud Maps at 2s, 4s, 6s, and 8s**

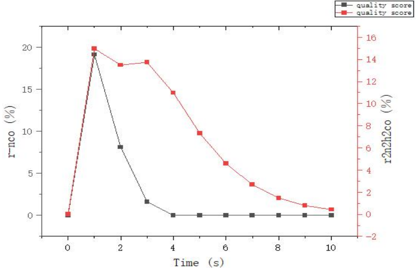


**Figure 8. Changes in Mass Fractions of Isocyanates and Polyurethanes at Reference Points**

As the temperature field increases, it can be clearly seen from the above data that the isocyanates in the control group react completely in the 6th second, while in the table with a temperature field of 340K, the reaction is complete in the 3rd second. Therefore, an increase in the volume of isocyanates can significantly increase the total reaction time.

## 4. Mechanical Properties of Polymer Products

The mechanical properties required for polymer grouting vary in different environments. In the working environment, the forces it experiences can be divided into tensile stress, compressive stress, and shear stress. Therefore, the study of the mechanical properties of polymer reaction products mainly focuses on the degree of deformation they undergo when subjected to tensile stress, compressive stress, and shear stress.

In order to facilitate simulation, the model is assumed to be fully elastic, homogeneous and isotropic. The polymer reaction product can be regarded as rigid polyurethane foam, and the mechanical properties are shown in Table 4.

**Table 4. Model Mechanical Attribute Settings**

| Attribute | Variable | value | unit | Attribute groups |
|---|---|---|---|---|
| Density | Rho | 42.6 | $Kg/m^3$ | essential |
| Young's modulus | E | 900000000 | Pa | Young's modulus and Poisson's ratio |
| Poisson's ratio | nu | 0.3 | 1 | Young's modulus and Poisson's ratio |
| Initial yield force | sigma | 300000 | Pa | Elastoplastic material model |
| Isotropic tangent modulus | Et | 200000000 | Pa | Elastoplastic material model |
| Tangent modulus of kinematics | Ek | 200000000 | Pa | Elastoplastic material model |
| Hardening function | sigma | 10000000 | Pa | Elastoplastic material model |

Due to the relatively hard nature and low deformability of rigid polyurethane, typically below 10%, the maximum deformation requirement for rigid polyurethane cannot exceed 10%. The abrasion resistance of polyurethane is affected by pressure. Test the deformation degree of rigid polyurethane, establish fixed constraints on the bottom of the cylindrical model using COMSOL software, and apply tensile stress, compressive stress, and shear stress along the positive z-axis direction at the top in sequence.

In summary, with a deformation degree of less than 10%, rigid polyurethane's maximum tensile stress is approximately 30000 N, the maximum compressive stress is approximately 30000 N, and the maximum shear stress is approximately 2000 N.

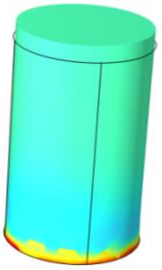


**Figure 9. Cloud Diagram of Tensile Stress on Cylindrical Body**

**Table 5. Tensile Stress Deformation Diagram of Cylinder**

| Number | Tensile stress N | Maximum displacement mm | Maximum deformation % |
|---|---|---|---|
| 1 | 10000 | 1.40 | 4.60 |
| 2 | 20000 | 2.20 | 7.30 |
| 3 | 30000 | 3.21 | 10.73 |

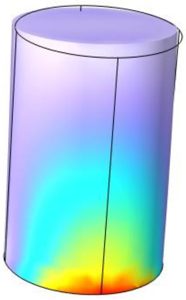


**Figure 10. Cloud Diagram of Shear Stress on a Cylinder**

**Table 6. Shear Deformation Diagram of Cylindrical Body**

| number | Shear force N | Maximum displacement mm | Maximum deformation % |
|---|---|---|---|
| 1 | 1000 | 1.70 | 5.70 |
| 2 | 1500 | 2.60 | 8.70 |
| 3 | 2000 | 3.40 | 11.30 |

## 5. Conclusion

This article focuses on the development needs of high polymer grouting technology in China, and adopts a combination of practical experiments and simulation analysis to study the flow characteristics and mechanical properties of high polymer polyurethane materials. The main achievements can be summarized as follows:

An experimental device for gel expansion of polymer slurry in a container is set up. The experimental setup for polymer slurry consists of a rectangular container, pressure sensor, thermometer, and syringe. The experimental device realized the reaction process of polymer slurry foaming in gel, and provided a practical experimental basis for conducting polymer numerical simulation and studying its diffusion mechanism.

The flow characteristics of polymers in gel foaming reaction and the mechanical properties of polymers under tensile stress, compressive stress and shear stress were simulated. The results showed that:

The increase in temperature field and the decrease in isocyanate volume can accelerate polymer reactions.

In the gel foaming reaction, the polymer is most affected by the ambient temperature, and the reaction is intense.

Polymers have strong compressive and tensile stress resistance, and weak shear stress resistance, but they can meet the daily use environme.

## Acknowledgments

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