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Modelling of impact of temperature gradient on content of polymer ampoule during its forming

G.M. Koloskova [a,*], V.Yu. Koloskov [b]

[a] Department of Theoretical Mechanics, Engineering Science and Robotics Systems, N. E. Zhukovsky National Aerospace University Kharkiv Aviation Institute, 17 Chkalova str., Kharkiv, 61070, Ukraine

[b] Department of Applied Mechanics and Environmental Protection Technologies, National University of Civil Defence of Ukraine, 94 Chernyshevska str., Kharkiv, 61023, Ukraine

* Corresponding e-mail address: g.koloskova@khai.edu

ORCID identifier: https://orcid.org/0000-0001-7118-0115 (G.M.K.); https://orcid.org/0000-0002-9844-1845 (V.Y.K.)

ABSTRACT

Purpose: The aim of the represented study was to model the impact of temperature gradient on content of polymer ampoule during its forming.

Design/methodology/approach: The model of polymer ampoules forming is built in SolidWorks software on the basis of finite element method. Using the developed model the study of temperature condition changes is carried out. Numerical modelling was carried out for two types of polymer packaging materials – polypropylene and polyvinylchloride – in similar conditions.

Findings: During polymer ampoule forming the highest temperature of liquid is obtained at the bottom of it. The most effective packaging method is to form the ampoule from polypropylene by means of aluminium die. Investigation results have shown that the highest obtained liquid temperature has linear dependence from initial one. Linear coefficients of heating were evaluated for polypropylene (equal to 0.72) and polyvinylchloride (equal to 0.58).

Practical implications: Decrease of initial liquid temperature value gives an opportunity to expand the range of products allowed to be packed in polymer ampoules in represented method. Safe conditions for packaging of liquid products in polymer ampoules are formulated, The results of the study may be used to improve the quality of liquid products packaging in polymer ampoules.

Originality/value: For the first time the model was developed for determination of liquid heating degree during its packaging in polymer ampoules. The calculations of the temperature distribution are represented for polypropylene and polyvinylchloride ampoules forming by means of aluminium and ceramic dies. The results of the study may be of interest to specialists in the field of polymer packaging manufacturing for food or pharmaceutical industry.

Keywords: Computational material science and mechanics, Polymer ampoule, Heating packaging method, Temperature modelling

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ANALYSIS AND MODELLING

1. Introduction

Today packaging and dosing systems are rapidly developed. New technologies allow creating various packaging equipment for different types of products [1]. An example of such packaging is represented with ampoules made of polymer and multilayer polymer films by means of heat forming method with simultaneous filling by product (see Fig. 1). Today they use such method to pack multiple range of medications and chemical substances. During sealing product contacts with heated walls of the ampoule, which may provide negative influence on product quality or even make it chemically or explosively dangerous without any visible changes. This circumstance has become a start for represented investigation.

Fig. 1. Thermally formed ampoules

In work [2] authors note that main tendencies of plastic packaging development at the legislative level dictate following requirements: 1) minimal migration of the components especially at increased temperatures of pasteurization and sterilization; 2) hot water durability which means form and sizes preservation; 3) high vertical loading durability; 4) high impact loading durability; 5) high transparency.

Therefore, investigations conducted in the field of existing polymer packaging materials we may divided in two sections.

First section represents investigations directed on provision of mechanical strength of packaging materials at different loading conditions. Almost all studies in these sections are based on experimental investigations [3]. Clear example of such study type is shown in work of author [4] dedicated to investigation of mechanical strength of T-shaped welded joint of polymeric films.

Second section includes investigations directed on provision of chemical strength of packaging materials, which means prevention of migration of packaging material components into the product or migration of product and packaging material components into environment. As most of packaging methods are connected with high temperature application, serious attention is paid to processes taking place during heating. For example, in work [5] authors have noted that increase of the temperature for 10°C intensifies biochemical reactions and lowers expiration date of the product. There are techniques allowing to calculate expiration date of main products [6], however there is no reliable criterion for evaluation of packaging suitability for product quality level preservation. For example, in work [7] authors have proposed to use variation of product anti-oxidant activity as such criterion. However, there are some products which anti-oxidant activity is varied only under high temperature impact despite of migrating components influence. For example, if honey is heated up to 43°C hydroxymethylfurfural is created in it. It is a dangerous toxic substance able to cause cancer formation in digestive tract [8]. And products containing aspartame sweetener cannot be heated over 30°C as it starts to disintegrate into formaldehyde and menthol [9].

Problem of certain components migration is important in other spheres too, for example, in sphere of technogenic safety provision [10]. In particular, in environmental safety provision sphere it is important to prevent penetration of nanoparticles into biosphere, which may lead to negative consequences [11]. In previous investigations it was found that nanoparticles immerse during utilization of polymer wastes [12] creates serious danger for surrounding environment, which causes necessity of application of special high-temperature disintegration technologies [13]. Yet, temperature regimes in polymer packaging, for example, during sealing taking into account packaging contents are not enough studied.

Energy efficiency provision during whole cycle of packaging taking into account all factors influencing usage and distribution of power is also topical task today [14,15].

Therefore, we may make a conclusion that results of investigations represented in modern publications do not give an opportunity to make generalized evaluation of the product heating during sealing of the polymer packaging. Perspective in this direction is application of mathematical modelling by means of finite element method. In their previous investigations authors have successfully used this approach for determination of parameters of honey heating during sealing in plastic cups [16], and for mechanical loading parameters evaluation during multi-layer combined materials forming [17].

The aim of the represented study was to model the impact of temperature gradient on content of polymer ampoule during its forming.

2. Materials and methods

Method of heat welding is based on polymer films heating and pressing by means of heated welding elements. As a result of heating the films are melted and adjoined with each other. Most often the heat welding is made by sealing element with constant or impulse heating.

Welding unit regularly consists of two aluminium or ceramic welding elements – lips – heated by means of heaters until polymer melting temperature is reached. Often they use profiled (ribbed) welding lips to raise heating surface. Additionally, this way it is possible to make more attractive weld.

In represented study, using SolidWorks software we have built 3D model of the system which forms ampoules (see Fig. 2). Lower forming blocks movement is provided by means of torque transfer from gear wheel to gear racks (see Fig. 2). Raising and lowering of welding blocks is provided by means of pneumatic systems in the back part of the system. Liquid is supplied from the tank to the exhaust heads by means of pneumocylinders.

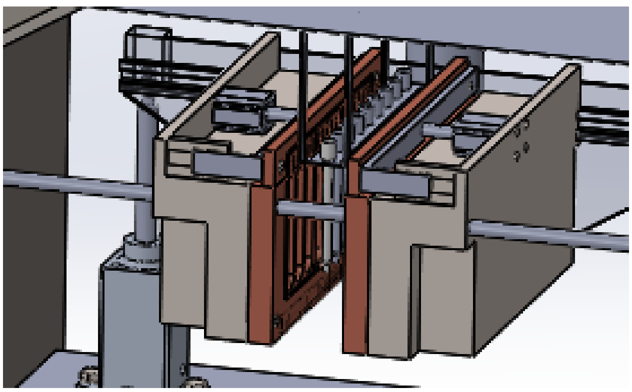

Fig. 2. 3D model of the system forming ampoules

Welding unit consists of easily replaceable rectangular die and heater (see Fig. 3). In represented study we have investigated two types of dies made of aluminium and ceramics. Physical-mechanical characteristics of die materials are shown in Table 1. Heating of forming blocks is provided by means of silicone adhesive plates put on the back side of the die. Heaters may have different configurations allowing to change temperature for various needs.

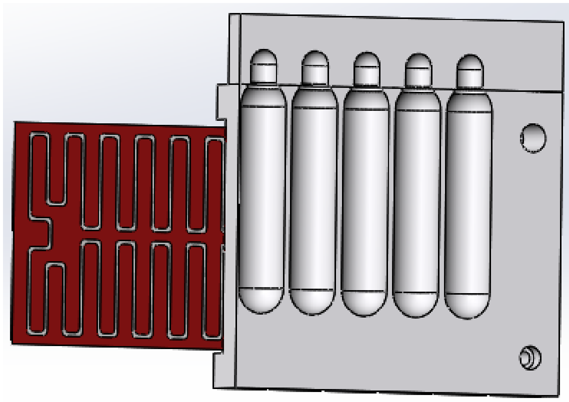

Fig. 3. Shape of the die with heater

We have investigated two types of ampoules produced of polypropylene and polyvinylchloride correspondingly. Polypropylene is widely used in packaging industry. Polyvinylchloride is one of the basic polymers, which is most widely spread in medicine sphere due to its chemical stability and inertness. Physical-mechanical characteristics of ampoule materials are shown in Table 2. Polymer film thickness is equal to 0.5 mm.

The process of ampoule forming consists of three stages. First, the film is moved between two lower die forms, which are pushed to each other. Melting temperature occurrence at stamp surfaces allows fast enough (average time is near 1 s) welding of the films, because for this it is necessary just to push together welding elements for the period of polymer crystallization.

The second stage includes forming of the ampoule by means of filling it with the product. Here the heater is switched off. The third stage includes forming of the ampoule head with the top die.

Simulation of the heating process for polymer film and product inside the ampoule was conducted by means of SolidWorks Simulation software.

The product material was simulated by distilled water with initial temperature equal to 293.15 K.

All external surfaces of die and heater have natural convection with heat transfer coefficient equal to 25 $W/m^2 \cdot K$. The surface, where ampoule forming takes place, has no convection as it becomes internal when die elements are connected.

Table 1.
Main physical-mechanical characteristics of die materials

Characteristic	Value	
Material name	Aluminium	Ceramics
Elastic modulus, Pa	$6.9 \cdot 10^{10}$	$2.2059 \cdot 10^{11}$
Poisson's ratio	0.33	0.22
Shear modulus, Pa	$2.6 \cdot 10^{10}$	$9.0407 \cdot 10^{10}$
Mass density, kg/m^3	2705	2300
Tensile strength, Pa	$11000 \cdot 10^4$	$17234 \cdot 10^4$
Coefficient of thermal expansion, 1/K	$2.36 \cdot 10^5$	$1.08 \cdot 10^5$
Heat conductivity, W/(m·K)	230	1.4949
Specific heat capacity, J/(kg·K)	900	877.96

Table 2.
Main physical-mechanical characteristics of ampoule materials

Characteristic	Value	
Material name	Polypropylene	Polyvinylchloride
Elastic modulus, Pa	$1.79 \cdot 10^9$	$2.41 \cdot 10^9$
Mass density, kg/m^3	933	1300
Tensile strength, Pa	$3300 \cdot 10^4$	$4070 \cdot 10^4$
Heat conductivity, W/(m·K)	0.117	0.147
Melting temperature, K	400-430	400-430

Simulation is carried out in two stages. The first stage is dedicated to finding of such system parameters as die temperature and heater temperature when polymer film melting temperature is reached. This condition marks forming of weld. The second stage is dedicated to ampoule filling with liquid. Here the influence of the temperature on ampoule content is studied.

In represented research we have investigated ampoules which volume is equal to 30 ml. Maximum filling time of such ampoules is 5 s.

3. Results and discussion

3.1. Results of temperature gradient modelling for ampoule forming by means of aluminium die

During polypropylene ampoule forming by means of aluminium die the film initial temperature at the sealing stage was equal to 293.15 K. Polypropylene melting temperature was reached in 1.3 s when initial die and heater temperatures were both equal to 443.15 K and heater power was equal to 1200 W. During this period the die temperature raised up to 439 K and heater temperature raised up to 441 K (see Fig. 4). These values are taken as initial conditions for following liquid heating calculation.

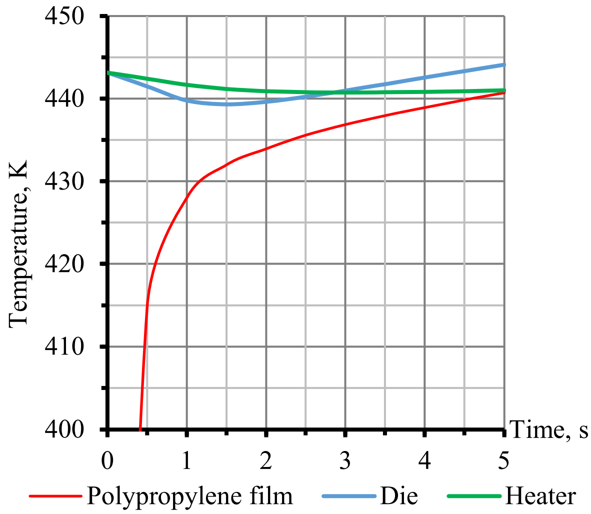

Fig. 4. Heating of the system elements when polypropylene ampoule is formed by means of aluminium die

Initial liquid temperature in ampoule is equal to 293.15 K. At this stage the heater is switched on which means that till this moment its power is equal to 0 W. Liquid is in ampoule which is pressed between two dies during 5 s. The liquid heating degree was observed in three places (on the side, in the centre and at the bottom of the ampoule). According to the chart of temperature distribution the place at the bottom of the ampoule corresponds to the highest temperature of the liquid (see Fig. 5). At given initial conditions sharp raise of the temperature occurs through the whole volume of the ampoule. Yet it is observed, that the water layers at the bottom of the ampoule were heated faster the centre ones (see Fig. 6). After that, the temperature redistribution takes place. Despite the increase of the side water layers temperature value it was observed that the temperature of in the centre of the ampoule start to decrease. This effect may be explained by ascending streams of hot liquid from below during its fast heating at initial stage. When heating from below comes to stable level, temperature redistribution takes place. The highest obtained temperature value in liquid is equal to 330 K, which is 37 K higher than the initial one.

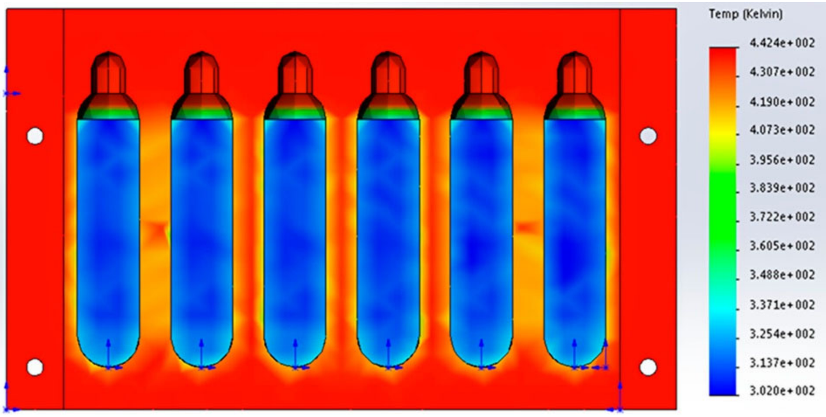

Fig. 5. The chart of temperature distribution for aluminium die and polypropylene film

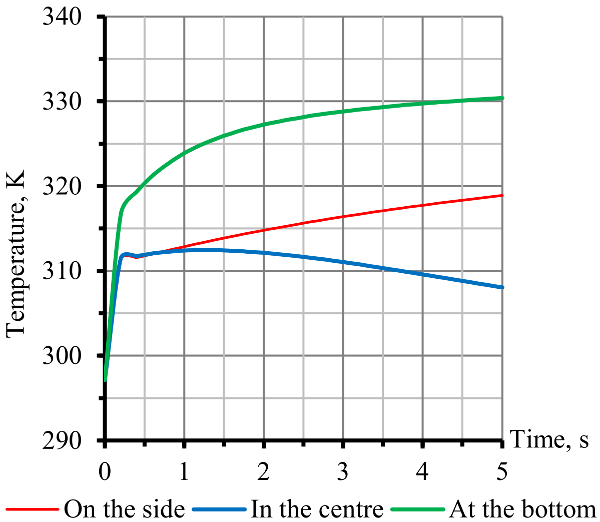

Fig. 6. Distribution of the temperature of liquid layers located in different places (on the side, in the centre and at the bottom) inside the polypropylene ampoule when aluminium die is used

During polyvinylchloride ampoule forming by means of aluminium die the film melting temperature was reached in 2.5 s when the die temperature raised up to 437 K and heater temperature raised up to 439 K (see Fig. 7). Same as for polypropylene case sharp raise of the temperature occurs through the whole volume of the ampoule and the water layers at the bottom of the ampoule were heated faster the centre ones (see Fig. 8).

However, at some point the temperature decreases in all places of the ampoule. It happens due to higher heat conductivity of polyvinylchloride in comparison with polypropylene. Thus, when intensive heat supply is over polyvinylchloride film is getting colder in much faster way. In addition, we may observe simultaneous decrease of the liquid temperature at the bottom and in the centre of the ampoule, which proves their connection. The highest obtained temperature value in liquid is equal to 351 K, which is 58 K higher than the initial one.

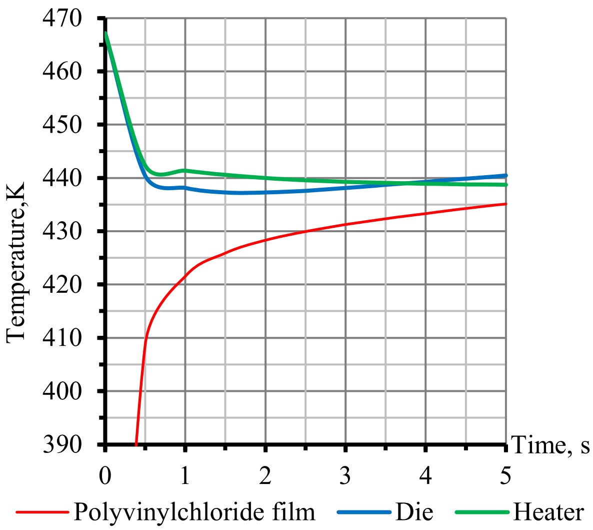

Fig. 7. Heating of the system elements when polyvinylchloride ampoule is formed by means of aluminium die

3.2. Results of temperature gradient modelling for ampoule manufacturing by means of ceramic die

Ceramics has very low heat conductivity in comparison with aluminium. However ceramic dies are widely used due their non-stick features shown in contact with polymers. For polypropylene ampoule initial conditions were following: polypropylene temperature is equal to 293.15 K, die and heater temperature both equal to 270 K, heater power is equal to 2000 W.

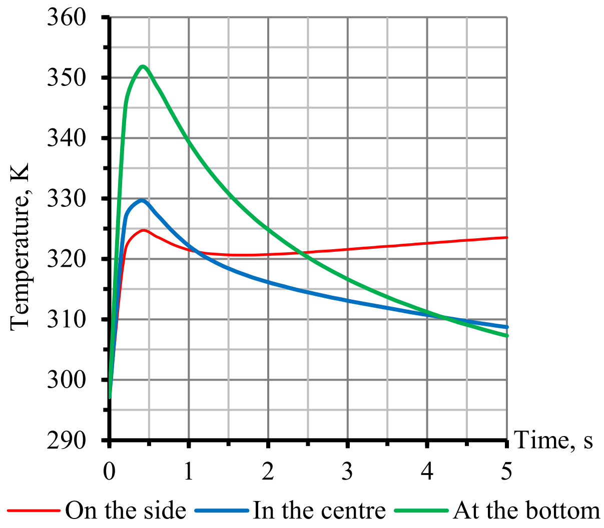

Fig. 8. Distribution of the temperature of liquid layers located in different places (on the side, in the centre and at the bottom) inside the polyvinylchloride ampoule when aluminium die is used

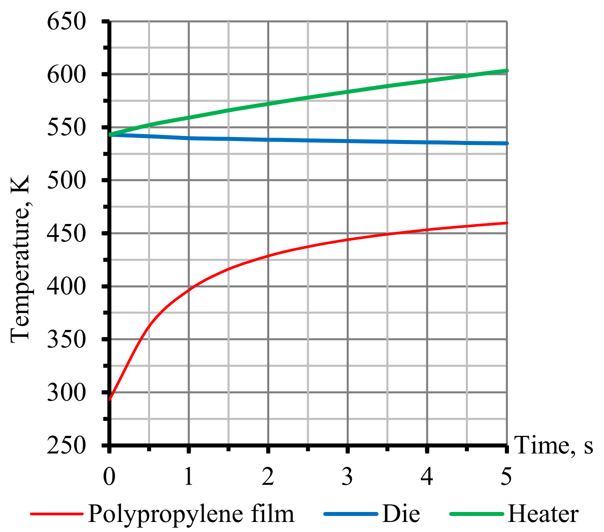

Fig. 9. Heating of the system elements when polypropylene ampoule is formed by means of ceramic die

Polypropylene melting temperature was reached in 3.8 s. During this period die temperature raised up to 533 K, and heater temperature raised up to 592 K (see Fig. 9). These values are taken as initial conditions for following liquid heating calculation.

Liquid heating process takes place in the same way as for aluminium die but at higher temperature (see Fig. 10). The highest liquid temperature is equal to 346 K which is 53 K higher than the initial one.

For polyvinylchloride at given initial conditions the melting temperature is reached within 6 s. Die temperature is equal to 610 K, heater temperature is equal to 717 K (see Fig. 11).

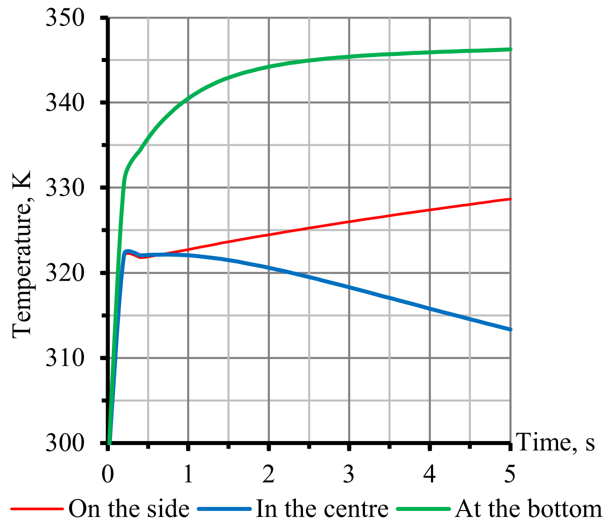

Fig. 10. Distribution of the temperature of liquid layers located in different places (on the side, in the centre and at the bottom) inside the polypropylene ampoule when ceramic die is used

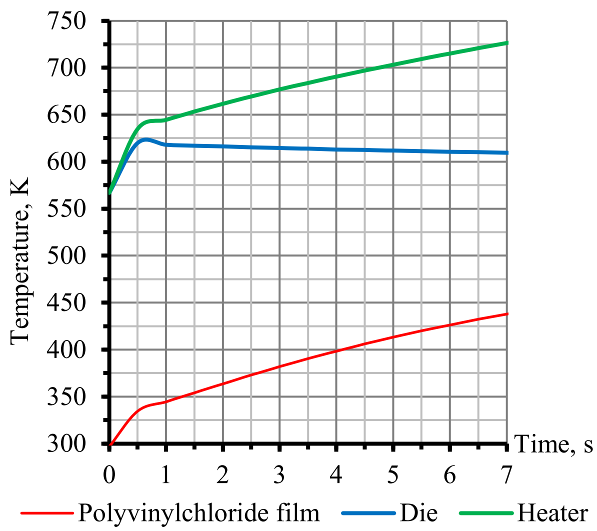

Fig. 11. Heating of the system elements when polyvinylchloride ampoule is formed by means of ceramic die

However, the behaviour of the liquid in polyvinylchloride ampoule (see Fig. 12) is similar to its behaviour in polypropylene one but at higher temperature.

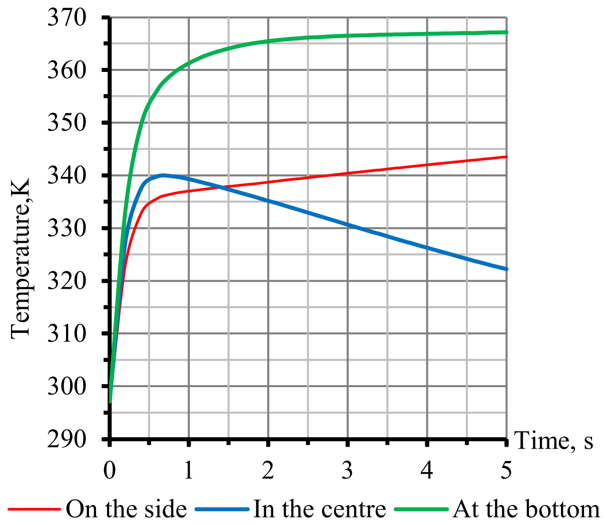

Fig. 12. Distribution of the temperature of liquid layers located in different places (on the side, in the centre and at the bottom) inside the polyvinylchloride ampoule when ceramic die is used

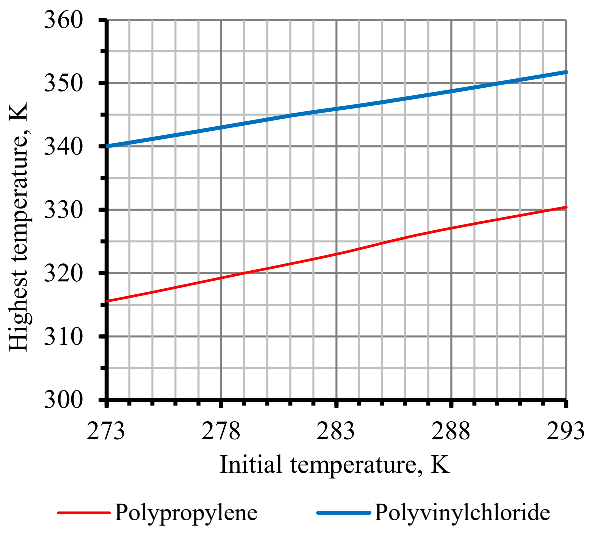

Fig. 13. Dependence of the highest obtained temperature of packed liquid from its initial value for polypropylene and polyvinylchloride ampoules

Fundamental difference occurring for the same ampoule material when different dies are used may be explained by the higher temperature of the die. Thus, the highest obtained temperature in the liquid in such case is equal to 367 K, which is 74 K higher than the initial one.

The most effective approach of all four observed ones is to use manufacturing of polypropylene ampoules by means of aluminium die because in this combination liquid is less heated. However, the temperature raise for 37 K in some cases may be dangerous. In addition, there are some occasions when polypropylene cannot be used. Following investigations were taken for both materials and aluminium die used.

To decrease heating temperature we have proposed lowering of the initial liquid temperature value. As it may be seen from the diagrams at Figure 13 temperature change takes place in accordance to linear law. Here linear coefficient of heating for polypropylene is equal to 0.72, when for polyvinylchloride it is equal to 0.58. Thus, we may state that polypropylene usage for ampoule manufacturing is more expedient as this material react better on initial liquid temperature decrease.

It should be noted that decrease of initial liquid temperature even to 273.15 K provides the highest obtained temperature equal to 315.56 K and 340 K for polypropylene and polyvinylchloride correspondingly. In turn, for surrounding temperature equal to 293.15 K it means the raise of the product temperature of 24 K and 46 K correspondingly, which in most cases is not appropriate.

4. Conclusions

As a result of represented research we have:

1. The model for determination of liquid heating degree during its packaging in polymer ampoules was built by means of SolidWorks Simulation software. Using this model the investigation of two types of ampoule materials (polypropylene and polyvinylchloride) used for forming by means of dies of two types of materials (aluminium and ceramics) was carried out.
2. Temperature variations in time of ampoule forming process were obtained for all ampoule and die materials combinations. It was found that the highest temperature values occur in the zone near the bottom of ampoule. For studied combinations of ampoule and die materials it was found that the most effective packaging method is to form the ampoule from polypropylene by means of aluminium die. In such case at initial liquid temperature of 293.15 K it will be heated for 37 K up to 330.15 K, which is destructive for some packed liquid products. Yet, maximum temperature difference between places in the centre and at the bottom of the ampoule is less than 30 K.
3. Investigation results have shown that the highest obtained liquid temperature has linear dependence from initial one. Linear coefficients of heating were evaluated for polypropylene (equal to 0.72) and polyvinylchloride (equal to 0.58). Thus, we have proposed to decrease initial liquid temperature value to expand the range of products allowed to be packed in polymer ampoules in represented method.

4. For the most effective ampoule and die materials combination "polypropylene–aluminium" when initial liquid temperature is decreased down to 273.15 K the highest obtained temperature is equal to 315 K which is fully appropriate.
5. Safe conditions for packaging of liquid products in polymer ampoules are as following: application of polypropylene ampoule and aluminium die combination; proper initial product temperature provision to grant safe highest temperature value; ability of the liquid product to keep temperature gradient up to 30 K without disintegration.

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