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NUMERICAL MODELING OF ACIDITY DISTRIBUTION IN ANTRODUODENUM AIMED AT IDENTIFYING ANOMALOUS ZONES AT CONSUMING DRINKS WITH DIFFERENT PH LEVEL

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The article focuses on describing mathematical model of a multi-phase flow in antroduodenum and its application for predicting digestive process features, including pH level detection. The suggested sub-model representing antroduodenal area of gastrointestinal tract is being developed within the frameworks of mathematical multilevel model depicting evolution of damage to critical organs and systems under exposure to risk factors. We introduced damages as per three functions (motor, secretory and absorbing one) to several gastrointestinal tract zones (body of stomach, antrum, and duodenum) and to pancreas and liver, into the sub-model. Mathematical problem statement includes records of mass and impulse conservation equations for mixture of liquid incompressible phases; ratios for mass flow intensity vector due to diffusion processes; ratios for mass sources due to reactions, secretion and components absorption, food dissolution, initial and terminal conditions. We obtained numeric experiment results when drinks with various pH level (2.3; 3.5; 7) were consumed; they revealed that anomalous considerable increase in acidity occurred in pyloric opening zone and duodenal cap zone when a drink with pH level equal to 2.3 was consumed. The results presented in this work make a considerable contribution into mathematical modeling development used to describe multiphase flows in biological channels with variable form. We showed that obtained acidity levels in various antroduodenum zones correspond to experimental data given in the works of other researchers. In future the model can be applied to predict risks of duodenum damages evolvement together with detecting areas of their localization under exposure to negative factors.

Key words: *mathematic modeling, functional damages evolution, antroduodenum, pH level, neutralization of acid, mucous tunic damages, tract motility, risk factors.*

Technologies and industrial productions are developing rapidly nowadays and it leads to greater volumes and wider spectrum of chemicals' emissions into the environment. Consequently, food stuffs can contain increased toxicants' concentrations, including heavy metals, which can penetrate, for example, vegetables and fruit via contaminated soil, atmospheric air, and water used for irrigation. Besides, manufacturers use new food additives to improve taste or to prolong storage life; however, impacts which are exerted on a body by such additives are not studied enough. Irregular and imbalanced

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nutrition also makes for additional risks for negative responses in terms of health; in particular, we can mention fast-food, fatty food and food rich in calories, beverages with increased acidity. For example, acidic content of gastrointestinal tract (GIT) can cause substantial damage to teeth enamel and dentin due to erosive factors [10, 13]; it can also cause ulcer evolvement in stomach and duodenum [20, 22].

The existing models applied for assessing influence exerted by environment on health as a rule are "black box models" and they don't apparently allow for variable exposure of factors, impact duration and mechanisms, organs and systems physiology [4, 9]. To get more profound insight into processes of damage evolving in organs and systems, a group of researchers, including the authors of this paper, offer to use a mathematic model based on multi-level approach [2]. The upper (or macro) level of the model deals with averaged interaction between organs and systems with the use of ordinary differential equations which describe damage evolution. Damage characterizes functional capabilities of an organ and it can be from 0 to 1 (0 means there are no functional disorders, 1 means that functions fail completely). Damage is assumed to change over time (age) due to natural aging processes and self-recovery processes in organs, non-normative intake of nutrients and chemicals, and medical treatment. Average (or meso) level is focused on physiology of a particular organ or system, damage mechanisms, interaction with other systems of a body. We should point out that at this stage sub-models of respiratory, digestive, and neuro-endocrine system at meso-level are being worked out [6, 8]. Later on it may become necessary to create models which will help to describe damage processes at cellular (or micro) level.

To solve tasks related to penetration of chemicals into a human body with food stuffs and drinking water, we are working out a digestive system model at meso-level [5]. This model is rather complicated and it requires additional sub-models creation to describe digestion and damage accumulation in various digestive organs and gastrointestinal tract sections more profoundly. This paper is dedicated to problems related to creating one of such mathematical sub-models describing physiological processes in antroduodenal section (antroduodenum) of gastrointestinal tract. It is this section where damage to mucous coat and ulcer evolvement occurs most frequently [1, 3], and it results from changes in balance between protection and damage mechanisms [22]. Increased acidity in the tract is one of the basic factors causing accumulation of damage in mucous coat; this increased acidity can be caused by various reasons, including insufficient alkali secretion for acid neutralization, defects in local bloodflow, and many other factors.

Direct measuring of acidity in gastrointestinal tract [11] has a number of disadvantages: it requires substantial time and material costs; measuring can be accomplished only in several points in certain moments, predicting is complicated, and an examined individual can suffer from unpleasant sensations. Besides, penetration of measuring devices into a human body can skew research results. In comparison with an experiment, mathematical approaches enable rapid changes in research design, including / excluding separate factors or conditions.

To consider space-distributed properties in gastrointestinal tract, it seems advisable to describe the examined processes with the use of multi-phase media mechanics techniques applying differential equations in partial derivatives. Mathematical models used for describing food flow in esophagus, [7, 25], stomach [14, 15, 18], and bowels [17, 16, 19], have been actively developed over the last decade. We should note that researchers, when developing models, as a rule consider tract motor function while biochemical reactions, digestive glands secretions, and food components absorption are given less attention. Comparatively few works deal with multi-phase modeling. Here realistic 3D shape of gastrointestinal tract sections and functional disorders occurrence, as well as food dissolution under hydrochloric acid and enzymes impacts, are not taken into account.

We accomplished conceptual and mathematical tasking, worked out algorithms of 3D shape reconstruction and tract motility as per ultrasound results, obtained some results on food dissolution speed at disorders in antroduodenum secretory function at previous stages of the research within the frameworks of the mathematical model which is described in this paper and deals with multi-phase flow in antroduodenum [26].

Our research goal was to examine acidity in antroduodenal section of gastrointestinal tract applying mathematical modeling in order to identify abnormal zones when consuming drinks with various pH level.

Data and methods. We studied multi-phase flow in antroduodenal section of gastrointestinal tract; in general, the first phase was multi-component liquid (water, pepsin, hydrochloric acid, sodium hydrogen carbonate, carbon dioxide, sodium chloride, dissolved complex proteins, fats, carbohydrates, polypeptides, and chemicals). Components were assumed to be dissolved at molecular level. To describe food, we used several liquid phases with various viscosity. Food particles were thought to have spherical shape in interphase interaction functions, phases differed as per dimensions ranges. Interphase interaction forces were considered to be proportional to differences in speeds of interacting phases.

Mass transfers from food phase into first phase components (water, dissolved proteins, fats, carbohydrates, and chemicals) under exposure to acid. Speed of interphase transfer depends on pH level of a medium, food dissolves only in acidic medium. Model allows for reaction of neutralization between acid and sodium hydrogen carbonate, and enzymatic reaction between pepsin and complex proteins.

We introduced damage to several sections of the tract into the model; these sections included body of a stomach, antrum, and duodenum; we also introduced damage to pancreas and liver which determined intensity of sodium hydrogen carbonate mass source in the area where ducts from these organs are located. Damage was defined as per each function, namely motor, secretory, and absorption one. We assumed that when motor function failed, it caused decrease in peristaltic wave amplitude in antrum and duodenum, and contractive capabilities of pyloric opening became weaker; when disorders in secretory function occurred, intensity of acid or alkali mass flow at the area boundary (tract walls) went down; in case of disorders in absorption function, mass outflow of chemicals became less intense.

The suggested model doesn't apparently allow for acid hypersecretion. Increased acid discharge is thought to be determined by regulatory mechanisms failure, or inadequate response to food stimulation. Only muscle weakness of circular layer in tract walls is considered among mechanisms which cause decrease in motor function; other disorders, for example, changes in contractions periodicity, are not taken into account. Lower toxicants absorption caused by damage to a tract wall can be explained by changes in mucous coat properties due to long-term exposure to a toxicant which is one of tolerance mechanisms. We should note that our model doesn't allow for dynamic changes in phases viscosity and density; nevertheless, phase properties in numeric experiments can be changed and we can analyze results which can correspond to, for example, various digestion stages in a stomach.

Speed of hydrochloric acid secretion is described by a dependence on average near-wall concentration of dissolved proteins, fats, and carbohydrates in a body of a stomach. Intensity of pepsin mass source is defined by dissolved proteins concentration. Physiological motive makes it advisable to use only near-wall concentration as receptors located in tract walls measure control element level and give a signal to control. The described regulation occurs locally as opposed to a signal to change intensity of sodium hydrogen carbonate mass source. Alkali secretion in antrum and duodenum as well as with pancreas and liver fluid depends on acid near-wall concentration in a body of a stomach and on neuro-endocrine system functionality responsible for giving a signal to control. The above-mentioned dependences are described with correlation with saturation similar to Michhaelis-Menten equation.

So, mathematical tasking includes record of mass conservation and impulse conservation equations for a mixture of liquid incompressible phases, correlations for the intensity vector of mass flow at the expense of diffusion processes, correlations for mass sources at the expense of reactions, secretion, and components absorption, food dissolution, initial and boundary conditions [26]. At a first approximation all the processes are thought to be isothermal, so mathematical tasking doesn't include temperature effects.

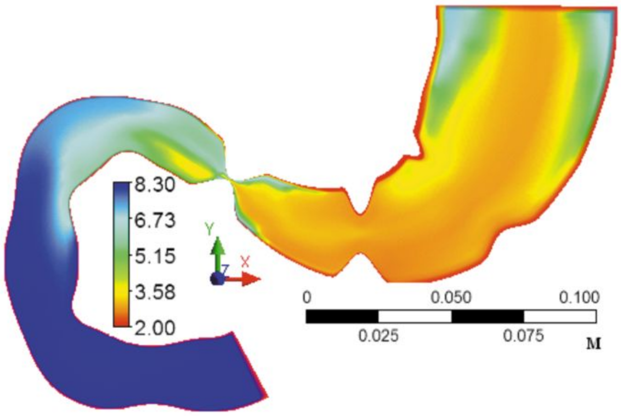
Results and discussion. We examined the effects caused by initially increased acidity (for example due to intake of acidic liquid) on dynamic distribution of acidity in antroduodenum. In this case the model became a bit simplified as we considered one-phase multi-component liquid (water, acid, sodium hydrogen carbonate, sodium chloride, and carbon dioxide).

At the initial moment of time increased acid concentration in stomach was set which corresponded to a beverage with a certain volume and acidity. The first scenario was focused on the case when a beverage with neutral acidity was consumed (pH = &) in a volume equal to 170 ml (for example, water). In the second scenario we analyzed acidity distribution in gastrointestinal tract when a beverage with increased acidity was consumed (pH = 3.5, volume equal to 170 ml), it could be, for example, apple juice, orange juice, any other fruit juice, or a fizzy beverage. In the third scenario we considered the case when a beverage with acidity (pH = 2.3) in a volume equal to 170 ml was consumed. Such acidity level is characteristic for lemon juice, Coca-Cola and other fizzy drinks [24].

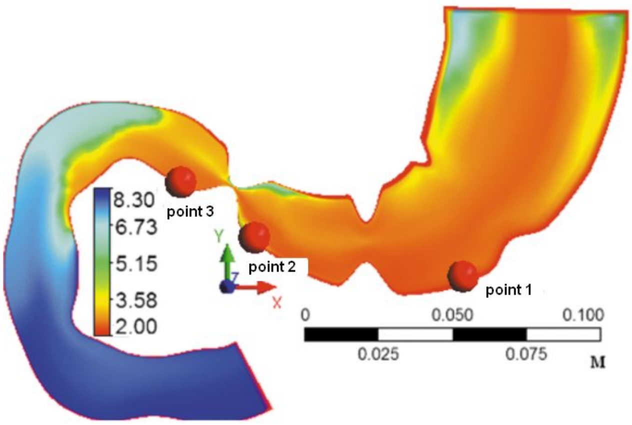
There were no functional disorders in antroduodenum in all three scenarios, in particular, intensity of hydrochloric acid secretion and sodium hydrogen carbonate secretion corresponded to the physiological standard observed in a healthy man.

If we analyze the results obtained in the first scenario, we can see that acidity in stomach cavity varies from 2.5 to 3.5 pH (figure 1, *a*). The parameters correspond to physiological standards. A zone with lower acidity (from 5 to 7 pH) occurs in near-wall layers of antrum and duodenum in order to provide protection from negative impacts.

In scenario 3 we can observe increased acidity in antroduodenum cavity (figure 1, *b*). Near-wall pH reaches 3 in the duodenal cap area and it can cause negative impacts on mucous coat of the tract. Three monitoring points are highlighted on figure 1, *b* in near-wall layer of stomach body (point 1), pyloric area (point 2), and duodenal cap (point 3).



a



б

Figure 1. Acidity distribution in the tract:
a – scenario 1, t = 330 s;
б – scenario 3, t = 330 s

In the first scenario we can observe that acidity in near-wall layers of stomach is within the physiological standard (figure 2, *a*). A slight increase in acidity occurs in pyloric area of stomach and duodenal cap area due to acidic content penetrating duodenum from stomach which is determined by increase in acid production intensity in response to stomach stretching.

In the second scenario pH level in near-wall layer of stomach and in pyloric area is close to values obtained in the first scenario when water was consumed (figure 2, *a*, *b*). In this case protection mechanisms of antrum mucous cost and pyloric area neutralize acid attack. pH in duodenum decreases to 4 during 5.5 minutes after a beverage intake due to acidic content penetration into bowels, and it remains substantially higher than the values obtained in scenario 3 (figure 2, *в*).

In the third scenario we can observe substantially increased acidity in pyloric area of stomach and duodenal cap area due to acidic beverage intake (figure 2, b, c). pH level in near-wall layer of stomach pyloric area starts to increase gradually (3 minutes after a beverage was consumed) and slowly due to acid neutralization and acidic beverage transfer into bowels. As a beverage comes into bowels in duodenal cap area, acidity remains substantially higher (2,3 pH).

On the whole we can note that if there are no functional disorders, sodium hydrogen carbonate neutralizes excessive acidity in antroduodenum more efficiently when a drink in a set volume with pH > 3.5 is consumed. Beverages with pH equal to 2.3 have much greater damaging potential for mucous coat of gastrointestinal tract walls as in scenario 3 acidity level in antroduodenum remained critically high during the whole estimated time. But if there is a disorder in alkali secretion, we can expect the area of potential damage to tract walls to be bigger. Acid negative impacts can reveal themselves in suppression of mucous coat cells capability to recover [23].

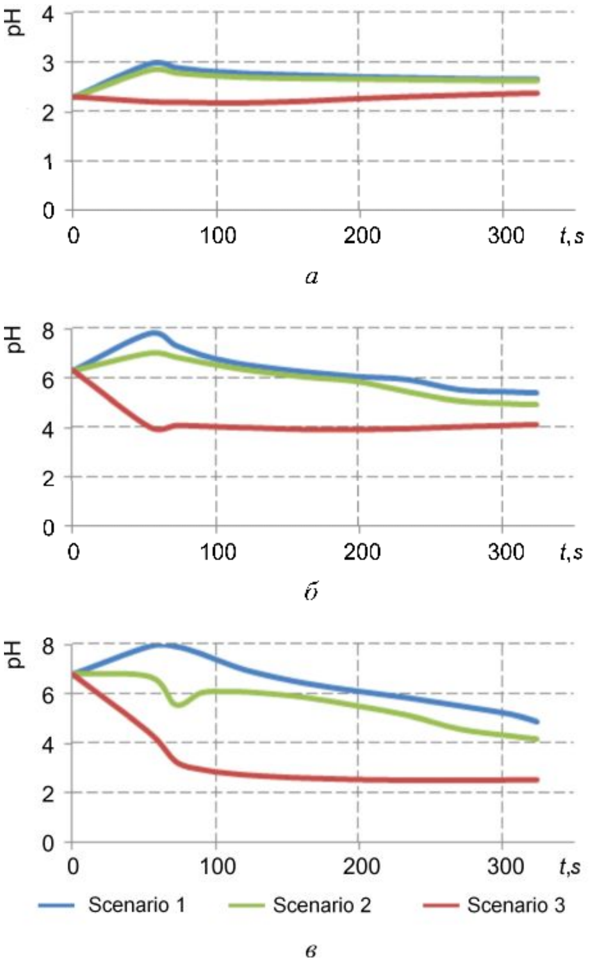


Figure 2. pH level dynamics near tract walls in various sections of it: *a* – body of stomach (point 1); *б* – pyloric area (point 2); *в* – duodenal cap (point 3)

The obtained results on acidity distribution in the tract coincide with the known experimental data: healthy people have pH level equal to 2.7 in body of stomach [12], and when Coca-Cola is consumed, a period of increased acidity in duodenum grows authentically [21].

Conclusions. The suggested mathematical model of multi-phase flow in antroduodenum can be used to highlight areas with abnormal increased acidity in pyloric area of bowels and duodenum depending on volume and pH of a consumed beverage.

Besides, in our further research we are planning to carry out numerical research on influence exerted by phases' viscosity and density, functional disorders occurrence, individual properties of tract shape and motility on features of multi-phase flow in antroduodenum area of gastrointestinal tract.

The results presented in this paper make a substantial contribution into development of mathematical modeling trend used for describing multi-phase flows in biological channels with complicated shape and moving boundaries, and with mass sources. A very promising trend in model development is identifying parameters of tract areas damage evolution due to acid impacts, self-recovery, and medical treatment. In this case the model can be applied for predicting risks for damage evolvement with detecting areas of its possible localizations. For more efficient practical use, it is advisable to extend range of diseases and disorders described by the model, as well as to add enzymes activity in it to get more detailed description of digestion processes in duodenum.

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