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A Stoichiometric Model of Human Metabolism

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Abstract. The present study deals with the "Human" component of the bioregenerative life support system. Here we develop a model that allows calculating metabolic mass flow rates of the "Human" component and monitoring the production of toxic substances – ammonia, hydrogen sulfide, and methanethiol. The model is designed as an Excel-VBA interactive program. The "Human" component is considered as an object with incoming and outgoing flows of matter. Food ingredients, water, and oxygen constitute the input flows, and the outgoing flows consist of metabolic products. The input flows are distributed along metabolic channels. To specify the characteristics of the "Human" component, a calorie counter and a space diet planner are connected to the model. The calorie counter is designed to determine a crewman's daily energy requirements depending on age, weight, height, gender, and level of physical activity. In turn, the numerical energy value is transmitted to the diet planner, which determines the food set. To more accurately present the metabolism of phosphorus, nucleic acids and phospholipids are included in the food composition. Each substance in the model is assigned a stoichiometric formula. The core of the model consists of seven stoichiometric equations and the water exchange unit, which are the link between the incoming and outgoing flows of matter. The solution of stoichiometric equations and balancing the water exchange unit are carried out using the Solver Add-in for Excel, which is embedded in the metabolic circuit. To show the validity of the model, a calculation of the human metabolism depending on calorie counter and diet planner is presented.

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Стехиометрическая модель метаболизма человека

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Аннотация. Объектом исследования является компонент «Человек», находящийся в биорегенеративной системе жизнеобеспечения. В данной работе разрабатывается модель, позволяющая рассчитывать метаболические массовые потоки компонента «Человек» и контролировать выработку токсичных веществ – аммиака, сероводорода и метантиола. Модель выполнена в виде интерактивной программы Excel-VBA. Компонент «Человек» рассматривается как объект с входящими и исходящими потоками вещества. Входные потоки составляют пищевые ингредиенты, вода и кислород, а исходящие – продукты метаболизма. Входные потоки распределяются по метаболическим каналам. Для задания характеристик компонента «Человек» к модели подключены счетчик калорий и космический планировщик диеты. Счетчик калорий предназначен для определения суточной потребности человека в энергии в зависимости от возраста, веса, роста, пола и уровня физической активности. В свою очередь, численное значение энергии передается в планировщик диеты, который определяет пищевой набор. Для более точного представления метаболизма фосфора в состав пищи включены нуклеиновые кислоты и фосфолипиды. Каждому веществу в модели присвоена стехиометрическая формула. Ядро модели составляют семь стехиометрических уравнений и блок водного обмена, которые являются связующим звеном между входящими и исходящими потоками вещества. Решение стехиометрических уравнений и балансировка блока водного обмена осуществляются с помощью надстройки Solver для Excel, которая встроена в метаболический контур. Для демонстрации обоснованности модели представлен расчет метаболизма человека в зависимости от счетчика калорий и планировщика диеты.

Ключевые слова: человек, метаболизм, моделирование, стехиометрические уравнения, космическое применение.

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Introduction

Since researchers began to model mass transfer in bioregenerative life support systems (BLSS), there has been a need to take into account human metabolism. This is an essential requirement because the human is the master component in the development of BLSS.

Complex circuits of human metabolism are known, including thousands of metabolites and metabolic reactions (Imielinski, Belta, 2010; Pantziri, Klapa, 2022). However, when modeling the "Human" component in BLSS, simplified stoichiometric models are used. It is assumed that simplification of the model does not lead to a major error in calculating human metabolism, and, consequently, in calculating the mass transfer in BLSS. Simplification of the scheme is achieved by minimizing the number of food ingredients and metabolic products, as well as the amount of controlled chemical elements. The minimum set of elements in stoichiometric formulas includes carbon, hydrogen, oxygen, and nitrogen. The variety of metabolic products is represented by generalized stoichiometric formulas (Belianin et al., 1980).

The functioning of the body becomes possible thanks to detoxification processes – the biochemical transformation and removal of toxic metabolic products. A metabolic model ignoring these processes would be incomplete. Toxic products – ammonia, hydrogen sulfide, and methanethiol – are formed during the anaerobic degradation of proteins in the intestine (Levitt et al., 1999). Therefore, this process should be included in the metabolic model. Stoichiometric models of human metabolism can have predictive power: based on them, mass transfer in the BLSS can be modeled before conducting an experiment. A feature of models of this class is their applicability only to the stationary state of human metabolism and mass transfer of BLSS in general.

This work aims to develop an interactive stoichiometric model of the "Human" component, which, with moderate complexity of the computer program, provides a more complete picture of metabolism compared with known models. The objectives of the work were:

- to provide a justification for the development of a stoichiometric model;
- to establish a connection between the stoichiometric model and the calorie counter and diet planner;
- to include anaerobic processes in modeling; and
- to construct a stoichiometric model taking into account the distribution of food ingredients along the input channels of metabolism and monitoring of toxic substances: ammonia, hydrogen sulfide, and methanethiol.

To facilitate understanding of the presented model, its description is given in the form of a specific example.

Rationale for constructing a model of human metabolism

Stoichiometric formulas in known models of human metabolism contain four chemical elements: carbon, hydrogen, oxygen, and nitrogen (Belianin et al., 1980; Volk, Rummel, 1987; Huttenbach, 1992; Hu et al., 2010). An exception is the model that includes sulfur and phosphorus in the model protein and, additionally, phosphorus in the nucleic acids (Manukovsky et al., 2005).

Limiting the number of biogenic elements to 4 is justified by the fact that biogenic elements C, H, O, and N have a predominant share in the circulating mass of BLSS (Table 1). However, the role of sulfur and phosphorus in the cycle of substances in BLSS is equally important. Knowledge of the nomenclature and quantity of sulfur- and phosphorus-containing metabolites at the output of the body can be useful in developing a method for their involvement in the material cycling. In the presented model, in addition to phosphoproteins and nucleic acids, phospholipids are introduced into the phosphorus metabolism scheme.

In addition to the models presented in Table 1, simplified metabolic balance schemes are described in other works (Ewert, Stromgren, 2019; Huttenbach, 1992; Calloway, 1975). However, they do not contain stoichiometric equations. Therefore, the numerical values of the incoming and outgoing flows of matter are not subject to change. The presented model contains the largest number of incoming flows of matter – 10 – and the largest number of stoichiometric equations – 7. Incoming flows relate to proteins, fats, carbohydrates, nucleic acids, phospholipids, fibers, ash, water consumed with food, oxygen, and water in the inhaled air.

Presumably, the inclusion of features 4–8 (Table 1) in the presented model will allow a more adequate expression of the metabolism of a particular crewman.

Table 1. Features of human metabolic models for space application

No	Feature	Models					
		Belianin et al., 1980	Volk, Rummel, 1987	Manukovsky et al., 2005	Hu et al., 2010	Vermeulen et al., 2023	Presented model
1	Number of input flows of matter	2	4	6	4	7	10
2	Number of stoichiometric equations	1	4	1	1	1	7
3	Number of controlled chemical elements in the formulas	4	4	6	4	4	6
4	Model's connection with diet	-	-	-	-	-	+
5	Distribution of food ingredients across metabolic channels	-	-	-	-	-	+
6	Accounting for anaerobic processes	-	-	-	-	-	+
7	Distribution of water and ash along the outgoing metabolic channels	-	-	-	-	-	+
8	Prompt replacement of formulas of model substances in the stoichiometric equations	-	-	-	-	-	+

+ presence of feature; – no feature.

Methods

Setting the initial data for calculating metabolism

The caloric value of the simulated food set was accepted as 2800 kcal according to a daily energy expense of crewman in the BIOS 3 system (Gitelson, Okladnikov, 1979) and simulated energy consumption of the inhabitant of a lunar base (Nitta, Ohya, 1991). To calculate the daily energy expense of a crewman, a calorie counter was designed (Fig. 1).

Using the calorie counter, a crewman's basal metabolic rate was determined taking into account age, weight, height, and gender. Then, daily energy requirements were calculated taking into account the level of physical activity.

As an example (Fig. 1), we established the following characteristics of a crewman: gender – "male", weight – 81 kg, height – 180 cm, activity level – "average", and the calculation formula – Mifflin-Geor (Mifflin et al., 1990). The calorie counter shows that in that case the daily energy consumption is about 2800 kcal.

The calculated caloric value of the food set is transmitted to the diet planner. The development of a diet is possible in two versions: in the form of a food set of ingredients (Kovalev et al., 2019) or in the form of a menu consisting of dishes prepared from a food set in a BLSS (Kovalev et al., 2020). In both options, a crewman's individual food preferences can be taken into account. The diet must meet the requirements developed for astronauts (Cooper et al., 2011).

Taking into account the established daily energy consumption of 2800 kcal and dietary requirements, the input of the model from the diet planner is 105 g of proteins, 97 g of lipids, 363 g of carbohydrates, 39 g of fiber, and 20 g of ash (Fig. 2).

The consumption of nucleic acids and phospholipids is not regulated by space nutrition standards. Therefore, daily consumption rates of

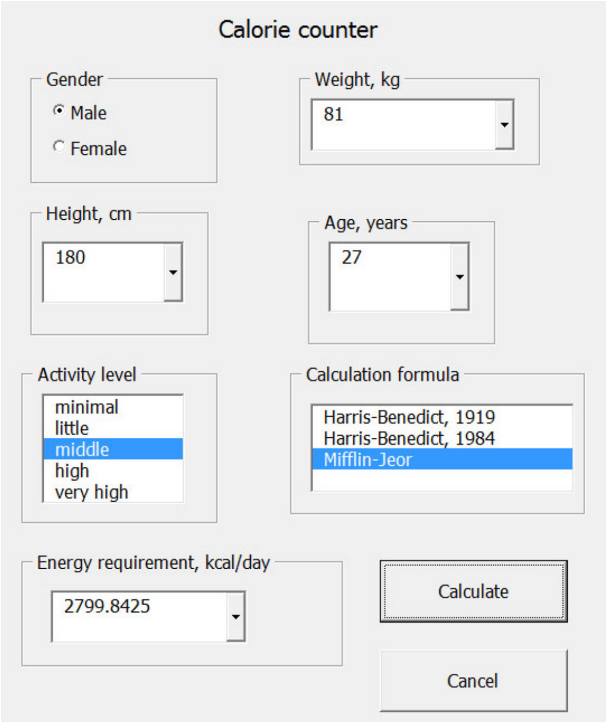

Fig. 1. Display of calorie counter

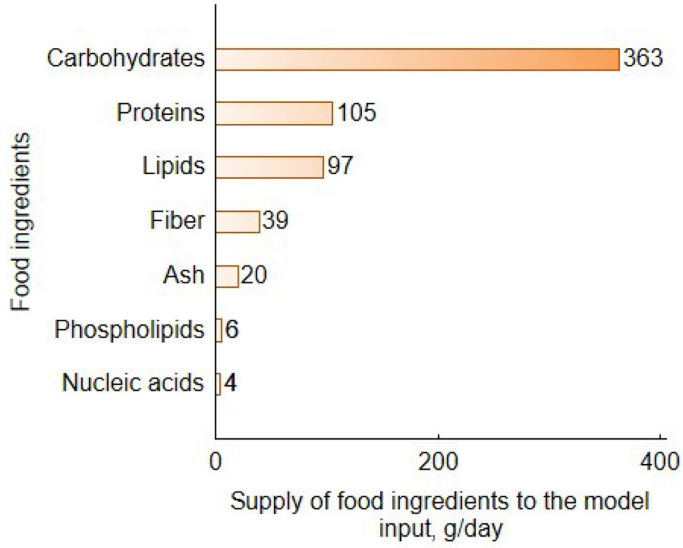

Fig. 2. Receipt of food ingredients from the diet planner to the simulated crewman

these ingredients are included in the model from the civilian diet (Cieślewicz et al., 2021; Cohn et al., 2010).

As part of foods, dishes, and drinks, a crewman receives 2271 g of water per day. An additional amount of water comes with the inhaled air. It was assumed that a crewman inhales 12 m^3 of air per day (Appendix 4, 2000), and the temperature and relative humidity of the air are 20 °C and 40 %, respectively (Korotcenkov, 2018). Under these conditions, a crewman inhales 84 g of water per day. The calculated daily masses of food ingredients and water from the diet planner are sent to the human metabolic model.

Metabolic input channels

The distributions of ingredients across metabolic channels are expressed as percentages. The sum of the percentages for each input substance is 100 %. Two types of processes occur in metabolic channels with incoming substances:

- chemical transformation, which is described by the stoichiometric equation with the subsequent distribution of metabolites into the metabolic output channels;
- the transfer of a portion of the input substance non-transformed into the metabolite.

The processes of the first type include, for example, the biochemical transformation of protein, fat, and carbohydrate with the participation of oxygen. The transition of protein, fat, carbohydrates, fiber, ash, and water into feces and miscellaneous substances (sebum, husks, cut hair, nails, and mucus) without chemical transformation belongs to the processes of the second type.

Balancing stoichiometric equations

When composing the equations, we used the formulas of model substances (Table 2). A by-product is a collection of organic products of protein metabolism (Belianin et al., 1980). The product formula was determined through chemical analysis of urine samples. In contrast, we calculated the generalized organic acid formula from the content of individual organic acids in feces (Morishima et al., 2021) using an empirical formula calculator (https://www.chemicalaid.com/tools/empiricalformula.php?hl=ru).

To calculate the coefficients of the stoichiometric equation, mass balance equations

Table 2. Empirical formulas of model substances used in the stoichiometric model

Model substances	Empirical formula in 1 C format	Reference
Protein (Casein)	$C_1H_{1.588}O_{0.311}N_{0.253}S_{0.005}P_{0.005}$	Calculated from Calloway, 1975
Lipid (Triolein)	$C_1H_{1.825}O_{0.105}$	Belianin et al., 1980
Carbohydrate	$C_1H_{1.667}O_{0.833}$	Vermeulen et al., 2023
Fiber	$C_1H_{1.667}O_{0.833}$	Hamad, 2021
Nucleic acid	$C_1H_{1.230}O_{0.726}N_{0.412}P_{0.104}$	Shchetinin, 2010
Phospholipid (Lecithin)	$C_1H_{1.833}O_{0.194}N_{0.028}P_{0.028}$	Ganeeva et al., 2016
By-product	$C_1H_{1.658}O_{0.360}N_{0.415}$	Belianin et al., 1980
Organic acid	$C_1H_{1.997}O_{0.834}$	Calculated from Morishima et al., 2021

were compiled for n chemical elements that make up m substances – reactants and reaction products (Poughon et al., 1997). The equations were solved using Excel functions – MINVERSE and MMULTIPLY.

When the condition m-n >1 was met, additional equations were introduced for the total number of balance equations to be m-1. Mass ratios between two selected substances were introduced into additional equations.

Additionally, Solver Add-in for Excel was built into the electronic metabolic circuit. The solver's objective function is the ratio between the daily masses of byproduct and urea in the stoichiometric equation of protein transformation. It was found to be 0.31 (Belianin et al., 1980).

Solver's purpose is:

- to solve balance equations containing mass relationships between two selected substances;
- to create a metabolic pattern that is consistent with experimental data (Semenov, 1971; Tolkachevskaya, 1940).

The independent variables of the solver are:

- mass ratios between two selected substances in additional balance equations;
- shares in the distribution of input substances;
- fiber digestibility coefficient;
- masses of water in urine, feces, and sweat.

The sum of the shares in the distribution of incoming substances is equal to 1. The fiber digestibility coefficient could vary within the range of 0.1–0.9.

Results and discussion

Proteins

Protein distribution occurs through three channels (Fig. 3). The share of proteins passed into feces is 10 %, according to (Calloway, 1975).

The "Miscellaneous transitions" channel receives 4 % of the total proteins, or 4 g/day. A significantly lower flow in this channel – 0.570 g/day – was noted in the work of Calloway et al. (1971). A list of components associated with this channel is known: skin cells – 3 g/day, hair – 0.33 g/day, saliva solids – 0.01 g/day, mucus – 0.4 g/day, and finger and toe nails – 0.01 g/day (Life support baseline values ..., 2022). Total: 3.75 g/day.

It is possible that proteins are distributed into the methanogenesis channel. A simplified description of protein degradation in this channel could be expressed as follows:

$$C_4H_5O_1N_1 + 3\ H_2O \rightarrow 2\ CH_4 + 2\ CO_2 + NH_3 \quad (1)$$

where $C_4H_5O_1N_1$ is formula of protein (Volk, Rummel, 1987).

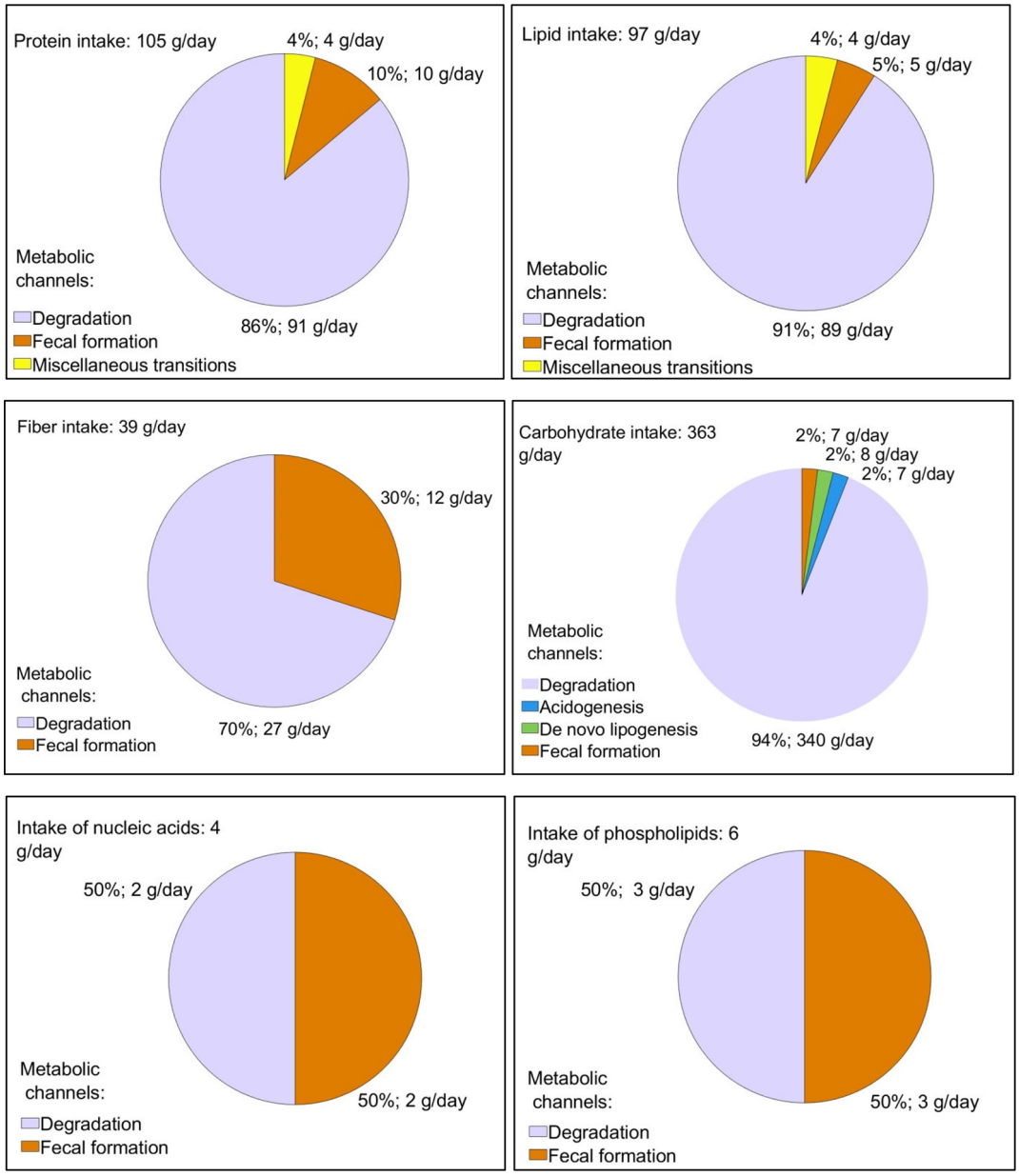

Fig. 3. Distribution of protein, lipids, fiber, carbohydrates, nucleic acids, and phospholipids at the model input along metabolic channels

In relation to this example of the presented model, we make the assumption that proteins are not distributed into this channel.

Protein degradation occurs under anaerobic and aerobic conditions. In the gastrointestinal tract, proteins undergo hydrolytic cleavage (Hucker, Carpenter, 1927). Some free amino acids are absorbed into the blood and transferred to the liver. There they undergo deamination to form organic acids and toxic ammonia (Bhagavan, 2002). Organic acids are transformed into pyruvate with the release of metabolic water. Pyruvate enters the Krebs cycle, in which carbon dioxide is formed (Litwack, 2021).

Ammonia is detoxified in the liver through involvement in the ornithine cycle to form non-toxic urea (Butterworth, 2019), which is removed from the body in urine (Putnam, 1971) and sweat (Keller et al., 2016). In addition to urea, urine contains a set of intermediate organic products of protein transformation (Belianin et al., 1980), having the general formula: $C_1H_{1.658}O_{0.360}N_{0.415}$.

However, not all ammonia is converted to urea, as evidenced by its presence in urine (Sarigul et al., 2019; Putnam, 1971), sweat (Ament et al., 1997), and feces (Clausen, Mortensen, 1992). Unlike other models of human metabolism (Belianin et al., 1980; Hu et al., 2010), in the presented model, ammonia is included as an end product. In addition to ammonia, urea, and by-products, the end products of protein transformation under aerobic conditions include carbon dioxide, metabolic water, sulfates, and phosphates (Belianin et al., 1980). The product of anaerobic protein conversion is hydrogen (Vermeulen et al., 2023), as well as hydrogen sulfide (Stummer et al., 2023), methanethiol (Tangerman, 2009) and thiosulfate, a product of hydrogen sulfide detoxification (Mimoun et al., 2012). With that said, the daily protein transformation looks like this:

$$\underset{\text{protein}}{4.010\ C_1H_{1.588}O_{0.311}N_{0.253}S_{0.005}P_{0.005}} + \underset{\text{metal ion}}{4.004\ O_2 + 0.103\ Me^{+}} \rightarrow 3.277\ CO_2 + 2.003\ H_2O + \underset{\text{by-product}}{0.311\ C_1H_{1.658}O_{0.360}N_{0.415}} + \underset{\text{urea}}{0.422\ C_1H_4O_1N_2} + 0.042\ NH_3 + 0.016\ H_2 + \underset{\text{thiosulfate}}{2.0E\text{-}05\ H_2S_2O_3} + 2.6E\text{-}07\ H_2S + \underset{\text{methanethiol}}{1.6E\text{-}08\ C_1H_4S_1} + \underset{\text{sulfate}}{0.020\ Me_2S_1O_4} + \underset{\text{phosphate}}{0.021\ Me_3P_1O_4} \quad (2)$$

Comparison of the calculated production of urea and ammonia with experimental data suggests that the calculated production falls within the range of variation of the experimental data (Table 3).

Table 3. Comparison of the calculated results with experimental data

Substances	Calculated production, g/day	Experimental data, g/day	Reference
Urea	25	20–35	Tolkachevskaya, 1940
Ammonia	0.7	0.4–1.2	Tolkachevskaya, 1940
Hydrogen	0.03	0.04	Kirk, 1949
Thiosulfate	0.002	0.002	Chwatko, Bald, 2009
Hydrogen sulfide	1.1E-06	9.0E-05	Kirk, 1949
Methanethiol	7.9E-07	8.5E-07	Sato et al., 2002

To estimate the production of hydrogen, thiosulfate, hydrogen sulfide, and methanethiol, it is necessary to know their maximum permissible production for a healthy individual. Insignificant production of hydrogen sulfide and methanethiol indicates their effective processing into sulfate and thiosulphate.

Lipids

Lipids at the input of the model are distributed over three metabolic channels (Fig. 3).

The largest amount of lipid undergoes oxidation:

$$5.710\ \underset{\text{lipid}}{C_1H_{1.825}O_{0.105}} + 8.014\ O_2 \rightarrow \rightarrow 5.710\ CO_2 + 5.210\ H_2O \quad (3)$$

5 % or 5 g/day of lipids pass into feces, according to Calloway (1975). 4 % or 4 g/day pass into sebum, which corresponds to experimental data (Life support baseline values …, 2022).

Fiber

The fibers are distributed along two input channels (Fig. 3). The Solver Add-in calculated the fiber digestibility coefficient as 0.7. This value is consistent with experimental data, where the digestibility coefficient varied within the range of 0.62–0.91 (Forsum et al., 1990). The indigestible part of the fibers is removed as part of the feces. The digestible part is subject to transformation, just like carbohydrates.

Carbohydrates

Carbohydrates coming from the diet planner are distributed into four metabolic channels (Fig. 3). Presumably, 25 g/day of digestible fiber enters the oxidative degradation channel, 1 g/day enters the acidogenesis channel, and 1 g/day enters the fecal formation channel. The largest part of carbohydrates and digestible fiber is oxidized to CO_2 and H_2O:

$$13.484\ \underset{\text{carbohydrate}}{C_1H_{1.667}O_{0.833}} + 13.484\ O_2 \rightarrow \rightarrow 13.484\ CO_2 + 11.237\ H_2O \quad (4)$$

The remaining amount of carbohydrates and digestible fiber is distributed into the processes of acidogenesis, fecal formation, and de novo lipogenesis (Ameer et al., 2014). Carbon dioxide, hydrogen, and methane are formed from carbohydrates as end products in acidogenesis. In addition to acetic acid, the human intestine contains propionic, butyric, succinic, lactic, isovaleric, valeric, and formic acids (Yokoyama et al., 2017). Hence, in equation (5), a summary formula of fecal organic acids is introduced. Combining the processes of acid formation and methanogenesis, we obtain the equation:

$$0.319\ \underset{\text{carbohydrate}}{C_1H_{1.667}O_{0.833}} + 0.338\ H_2O \rightarrow \rightarrow 0.290\ CO_2 + 0.574\ H_2 + 0.0003\ CH_4 + 0.029\ \underset{\text{organic acid}}{C_1H_{1.997}O_{0.834}} \quad (5)$$

Methane production is not observed in all people (Kirk, 1949). Acetic acid can be a precursor to methane (Kostryukova, 2019). However, the major amount of methane is formed during the reduction of carbon dioxide by hydrogen (Weaver et al., 1986).

When determining the proportion of carbohydrate that turns into fat, we relied on the work by Volk, Rummel (1987). From this work it can be calculated that about 2 % of carbohydrates are transformed into fat. The stoichiometric equation for de novo lipogenesis in the presented model is as follows:

$$0.308\ \underset{\text{carbohydrate}}{C_1H_{1.667}O_{0.833}} + 0.024\ H_2O \rightarrow \rightarrow 0.308\ \underset{\text{lipid}}{C_1H_{1.825}O_{0.105}} + 0.124\ O_2 \quad (6)$$

The reverse process of transformation of fats into carbohydrates is known (Landau, Brunengraber, 1987). This process is not considered in our work.

Nucleic acids

Nucleic acids are distributed along 2 metabolic channels (Fig. 3). Presumably, a

fraction of 0.5 becomes part of the intestinal microflora, and a fraction of 0.5 is converted into metabolic products.

The initial stage of degradation is carried out with the help of nucleases from the pancreas and small intestine (Yang, 2011). Purine and pyrimidine degradation ends in the formation of carbon dioxide, urea, and uric acid (Kaneko et al., 2014). Metabolic water and small amounts of ammonia may be formed. Summarizing the above, we obtain the equation for nucleic acid degradation:

$$0.059\ \underset{\text{nucleic acid}}{C_1H_{1.230}O_{0.726}N_{0.412}P_{0.104}} + 0.047\ O_2 + \\ + 0.018\ \underset{\text{metal ion}}{Me^+} \rightarrow 0.040\ CO_2 + 0.014\ H_2O + \\ + 0.009\ \underset{\text{uric acid}}{C_1H_{0.800}O_{0.800}N_{0.600}} + 0.009\ \underset{\text{urea}}{C_1H_4O_1N_2} + \\ + 0.00001\ NH_3 + 0.006\ Me_3PO_4 \quad (7)$$

Phospholipids

The normal dietary intake of phospholipids is known to be 2–8 g/day (Cohn et al., 2010). Therefore, we select 6 g/day, which is within the range indicated above. Presumably, phospholipids are distributed in equal proportions along two metabolic channels (Fig. 3). One part passes into feces, and the other part undergoes degradation.

Lecithin was used as a model phospholipid in the calculations (Table 2). Phospholipases break down lecithin into phosphatidic acid and choline (Fisher, Jain, 2009).

Hydrolysis of phosphatidic acid produces fatty acids with one and two molecules of glycerol and phosphate, respectively (Athenstaedt, Daum, 1999). Glycerol can undergo oxidation to form CO_2 and water (EFSA ANS Panel et al., 2017).

Choline is involved in the sequence of transformations: choline – betaine – dimethylglycine – sarcosine – glycine – serine (Dobrijevic et al., 2023). Serine is converted to pyruvate, releasing ammonia (Beltrán-Castillo et al., 2018). Pyruvate is included in the Krebs cycle, which produces CO_2 and water (Roosterman, Cottrell, 2023). Ammonium is converted to urea (Butterworth, 2019). Ammonia residues and urea are excreted from the body in urine and sweat (Tolkachevskaya, 1940). The equation describing the catabolism of lecithin to form end products is as follows:

$$0.170\ \underset{\text{lecithin}}{C_1H_{1.833}O_{0.194}N_{0.028}P_{0.028}} + 0.238\ O_2 + \\ + 0.015\ \underset{\text{metal ion}}{Me^+} \rightarrow 0.168\ CO_2 + 0.151\ H_2O + \\ + 0.002\ C_1H_4O_1N_2 + 0.00005\ NH_3 + \\ + 0.005\ Me_3PO_4 \quad (8)$$

Ash

Presumably, ash is not involved in biochemical transformations (Fig. 4). Ash distribution is limited by its concentration in urine, feces, and sweat.

Water balance

Metabolic water is attached to the water consumed and inhaled (Fig. 5). In total, 2690 g of water per day is supplied to the model input. The same amount of water is released from the body (Fig. 4). The data reported by Shibanov (2007) served as a guide to the distribution of water along the metabolic output channels.

Some water is removed from the body through the process of flatulence. To estimate this amount, we assumed that the air flow during flatulence is 1.48 ml/min (Kirk, 1949), and the mass of water in 1 m^3 at a temperature of 35 °C and a relative humidity of 90 % is 37.9 g (https://airwet.ru/tpost/o7gzpmlts1-skolko-grammov-vodi-soderzhitsya-v-1-kub). Then only 0.08 g of water per day is released through the anus. Therefore, this flow is not taken into account.

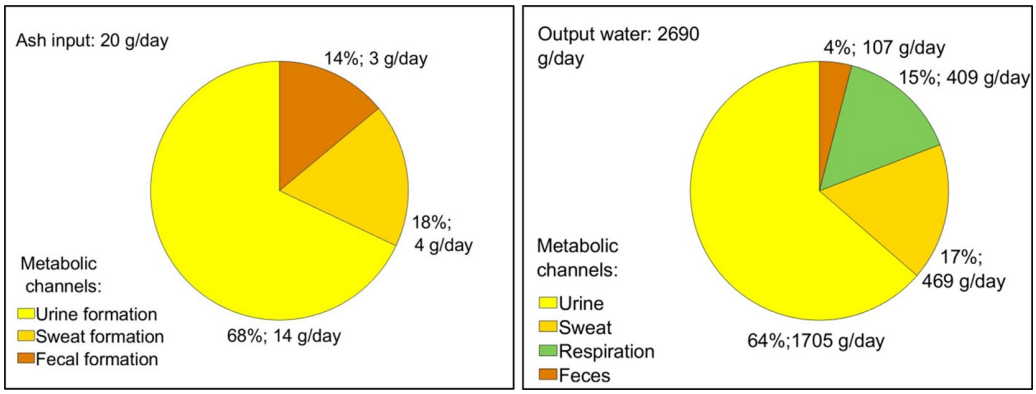

Fig. 4. Distribution of ash and water at the model output along metabolic channels

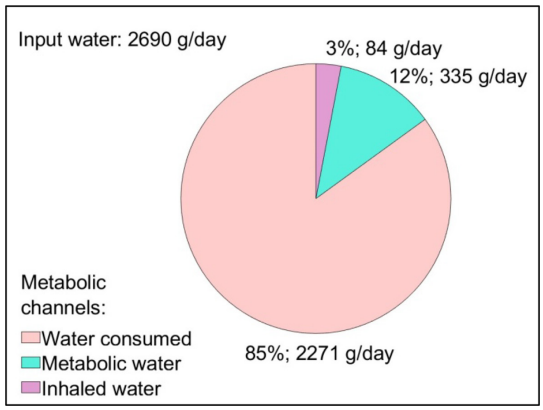

Fig. 5. Water sources at the model input

Total balance

One can see that the flows of carbon dioxide and oxygen dominate human metabolism (Fig. 6). Therefore, even a slight change in the stoichiometric formulas of substances that are sources of carbon dioxide can lead to a significant change in its calculated production. As noted above, the presented model allows one to quickly change the stoichiometric formulas of substances. Here we will consider replacing the carbohydrate formula (Table 2) with the formula used in the stoichiometric BLSS model (Volk, Rummel, 1987): $C_1H_2O_1$.

The replacement leads to a decrease in carbon dioxide production to 950 g/day and a decrease in oxygen consumption to 778 g/day. To avoid significant errors in predicting human and BLSS metabolism, the stoichiometric formula of the carbohydrate component of food should be determined as accurately as possible.

Metabolism modeling should ultimately lead to obtaining parameters of urine, feces and sweat that would not go beyond the experimental data. The obtained parameters of human secretions (Table 4) do not contradict known experimental data (Wignarajah et al., 2006; Human…, 1975; Semenov, 1971; Tolkachevskaya, 1940).

Conclusion

An interactive and person-specific stoichiometric metabolic model has been

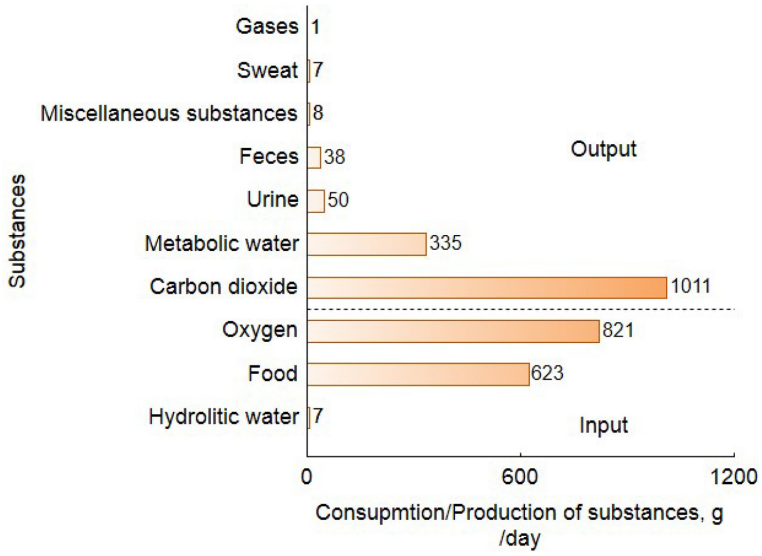

Fig. 6. "Input-output" balance of stoichiometric model

Table 4. Calculated parameters of urine, feces, and sweat

Parameters	Urine	Feces	Sweat
Water, %	97	74	98
Organics, %	2	24	1
Ash, %	1	2	1
Output, g/day	1767	145	476

developed. The model is intended for calculating human mass transfer as a component of a bioregenerative life support system, but in the future it may become a tool for developing an astronaut's medical passport. At the same time, the present study revealed problems in metabolism modeling. These include uncertainties in the distribution of substances along metabolic channels and the identification of conditions for reliable detoxification of the body. A necessary continuation of the work should be the development of a dynamic model of human metabolism, taking into account the results of stoichiometric modeling.

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