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MASS BALANCES FOR A BIOLOGICAL LIFE SUPPORT SYSTEM SIMULATION MODEL

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ABSTRACT

Design decisions to aid the development of future space-based biological life support systems (BLSS) can be made with simulation models. Here we develop the biochemical stoichiometry for 1) protein, carbohydrate, fat, fiber, and lignin production in the edible and inedible parts of plants; 2) food consumption and production of organic solids in urine, feces, and wash water by the humans; and 3) operation of the waste processor. Flux values for all components are derived for a steady-state system with wheat as the sole food source. The large-scale dynamics of a materially-closed (BLSS) computer model is described in a companion paper /1/. An extension of this methodology can explore multi-food systems and more complex biochemical dynamics while maintaining whole-system closure as a focus.

INTRODUCTION

Until actual closed systems with humans are built and tested, mathematical models utilizing empirical knowledge of components will be the only means available to test hypotheses regarding the operation of these systems, particularly regarding those properties characteristic of the system-as-a-whole. Such models have been important in the research towards biological life support systems /2-4/. Averner /2/ developed the concept of elemental balanced here extended to generalized stoichiometry. Others /3,4/ investigated the influence of feedback controls on recovery following a waste processor failure, illustrating the potential for complex whole-system dynamics. Our intent is to simulate a system that embodies current understandings of space station module volumes, experimental plant growth results, human metabolism, etc., to produce a model that provides information regarding the flow dynamics of a space-based BLSS.

In a companion paper /1/ we develop a mathematical simulation of a closed system that will be able to approach whole-system issues, such as the need for reservoirs and buffers /5/. Biological models at the ecosystem level /6/, the whole-person level /7/, the whole-plant level /8/, the plant-part (leaf) level /9/ are appropriate for other specific inquiries. An awareness that different structural/functional levels possess different properties that may not be obvious from any other level /10/ is essential. Therefore our focus is on the whole system for potential applications for space life support. This system is constructed from major components, such as the plant growth module, the crew compartment, and the waste and environmental controls, each of which are in turn complex systems with internal dynamical parts. This paper examines these systems on the biochemical level in order to develop stoichiometric relations governing the material flows in the system model /1/, focusing on the elements that constitute most of the system's mass: carbon (C), hydrogen (H), oxygen (O), and nitrogen (N). More complex processes can be incorporated in the future, but rather than constructing any particular component in great detail, our aim is to first construct an entire operational model system that is capable of further and diverse modification.

THE COMPONENTS

The Plants

The three general categories of food type -- proteins, carbohydrates, and fats /11/ -- are metaboloids. Although a vast plethora of substances are manufactured by plants, we take the triad of protein, carbohydrate, and fat as important substance-types to track in the model. This necessitates plant species-specific equations that convert carbon dioxide (CO₂), water (H₂O), and a nitrogen source into these food types. These equations are now developed, along with reasons for choosing particular canonical formulas, which are summarized in Table 1.

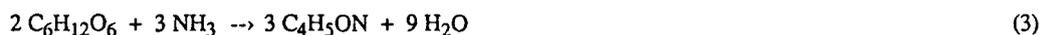
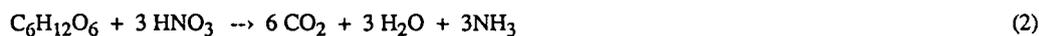
Carbohydrate. Photosynthesis, most simply expressed, creates glucose and free oxygen from carbon dioxide and water by



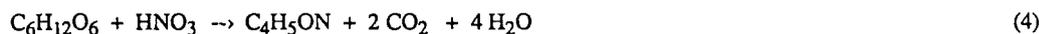
This reaction has a Gibb's Free Energy change of +686 kcal /12/ and therefore C₆H₁₂O₆ contains energy that can be used to drive other reactions in the plant. Glucose, the most abundant monosaccharide, is the parent from which most others are built, including the much larger polysaccharides /12/.

Protein. To obtain a representative canonical protein, the 20 amino acids present in most proteins /13/ are first averaged by calculating the CHON mass fractions for each amino acid and then averaging the twenty C-fractions, H-fractions, etc. For this procedure to be perfectly valid, the 20 amino acids should be equally abundant in terms of mass in proteins, which is not the case for any particular protein, but is reasonable for a range of proteins over a range of organisms. The average obtained is listed in Table 1 as "mass av'd amino acid". Another possible way of averaging is to assume the different amino acids are present in proteins in approximately equal numbers; this average is obtained by summing the C-atoms, H-atoms, etc. in all 20 amino acids and then dividing by twenty. This method results in "no. av'd amino acid" in Table 1, with its CHON fractions very similar to those from mass-averaging.

A simple formula that approximates these empirical element distributions is $C_4H_7O_2N$, shown in Table 1. Proteins, in turn, are formed by chaining amino acids through peptide bonds /13/, which effectively removes an H_2O from each amino acid. Therefore, rather than using the average amino acid as protein, a protein formula is better represented by C_4H_5ON , which gives a N-content close to the 16% found in typical proteins /11/. Therefore the reduction of nitrogen from nitrate to ammonia and its incorporation into protein during biosynthesis from carbohydrate (hexose) is written



Equations (2) and (3) can be added,



Fat. The category fat is taken here to include all substances in the ether extract of a Weende analysis /11/, for example, fatty acids, waxes, and phosphoglycerides. They are all characterized by low amounts of O (and zero N) relative to C and H, and are therefore similar in structure. Palmitic and stearic are most common saturated fatty acids found in both animal and vegetable fat /14/. Palmitic ($C_{15}H_{31}COOH$) will be taken as the canonical fat with CHON fractions listed in Table 1 and formed by biosynthesis from carbohydrate by



The energy needed to form fat and any other plant product is not explicitly accounted for in these equations, for the reverse reaction of equation (1) or similar respiration processes would have to occur along with equation (4). Respiration does not contribute to the mass of the plant, which is the focus here, but is important in the system simulation /1/.

Fiber. Plant fiber is important in a simulation model because there will be inedible parts of the plant, primarily because of the presence of large, linked polysaccharides that inhibit digestibility /11/. These are usually considered separately from the even less digestible lignins (see below). Although the fibers have a complex biochemistry that includes hemicelluloses, celluloses, and xylans /15/, cellulose as the basic structural material of cell walls in all higher land plants will be the representative fiber, with formula $(C_6H_{10}O_5)_n$ /11,16/



Lignin. The final important plant component is taken to be lignin because of its ability to appreciably reduce digestibility in small amounts /11/ and is usually found associated with the fibrous materials. A typical lignin is characterized by chains of $C_{10}H_{11}O_2$ (11) and can be formed by

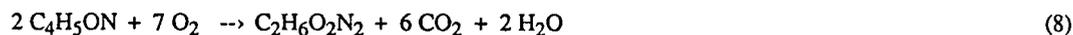


The Humans

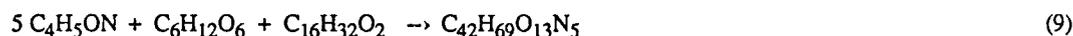
Respiration and waste solids. Humans consume food containing protein, carbohydrates, and fats defined by the same canonical formulas produced by the plants. A fraction of the carbohydrates and fats are assumed to be completely respired to form CO_2 and H_2O by reversing equations (1) and (4). Humans also produce organic solid wastes of different types than found in foods. These -- urine, feces, and wash water solids -- will now be considered.

Urine solids. Human urine has on the order of 25 organic constituents /17/ whose concentrations each exceeds 50 mg/l. Urea ($(NH_2)_2CO$) is by far the most abundant /12,17/, with well over 50% of the total organic solids, followed by much smaller amounts of creatinine, uric acid, ammonia, and still smaller amounts of phenols and oxalates /18/. The CHON fractions of urea and of urine solids given calculated from Lehninger's listing of compounds /12/ is shown in Table 1; it would appear that urine solids are essentially urea. However, a substantially different distribution with more O and less N appears in the elemental listing measured from a standardized freeze-dried urine samples /19/, which is also shown for comparison in Table 1. We obtained a value for the unlisted O in this reference by subtracting the sum of the 15 elements listed from a total of 100%. The reason for these CHON differences is not apparent.

The most complete listing of compounds and CHON fractions for categories of compounds is that of Putnam /17/, whose total O and N for organic solids are between those values from references /12/ and /19/; see Table 1. This study /17/ notes that the formula $C_2H_6O_2N_2$ approximates the CHON distribution of urine solids. This formula can be re-structured as urea plus a sugar precursor ($(NH_2)_2CO + CH_2O$). Although significant glucose in urine is characteristic of a pathology /18/, the many nitrogenous compounds other than urea that exist in urine and the concentrations of the non-nitrogenous compounds happen to produce the above average urine compound, whose urea percentage of the total is a reasonable 67%. Excretion of urea is a principle method the body has to rid itself of ammonium ions in the blood and tissues, and this urea is formed by the hydrolysis of arginine to ornithine /18/. Since arginine can be synthesized and the pathways are more complex than we need for the BLSS system at this point, we will take the formation of urine solids ($C_2H_6O_2N_2$) from the generalized protein to be



Feces solids. Table 1 lists the CHON fractions from two sources /16, 19/, in which the latter's O was obtained by difference from the table listing elemental composition of freeze-dried feces. The differences between the two sources is perhaps not too surprising given that feces is almost as varied as the food that is eaten. However, following the procedure for urine solids to include some recognition of the composition, Orten and Neuhaus /18/ note that the dry content of feces is 25-50% dead and living bacteria; bacteria are about 50% protein /20/. Feces is an important export for fats from dietary by-products or undigested lipids, and lipids of various types can constitute up to 33% of the dry mass of feces /18/. Other undigested, indigestible or unabsorbed food residues are found. As a possible feces solids composition we take 50% protein (25% from bacteria, 25% undigested food), 25% fat, and 25% carbohydrate. The carbohydrate is not intended to represent undigested glucose, but rather serve as a proxy for undigested non-nitrogenous plant matter. Using the formulas for protein, fat, and carbohydrate above, this mass distribution is approximated by



This produces CHON fractions generally between those of the two references and will therefore be taken as reasonable. The concern with the substances that comprise urine and feces solids is motivated by the requirement that the BLSS system model should ultimately contain feedbacks within the system. Ultimately, rather than specifying the amounts of urine and feces solids produced each day, they should be linked to the composition of the food eaten. This will be facilitated by deriving some of the reasons behind the CHON fractions of these solids. The same goes for wash water solids.

Wash water solids. Wash solids consist of residues primarily from the skin's surface during washing, and are listed as sweat solids, an important organic solids constituent to be considered along with urine solids and feces solids in designing space life support systems /21/. The composition of wash water solids has been studied /16/ and is displayed in Table 1, both including and excluding soap from the organics. Since the model is not recycling soap at this point, we will exclude soap (about 30% of the total organics) from consideration. The remaining constituents are lactic acid, urea, glucose, and unknown insolubles. From the analysis and assumptions in reference /16/ about 15% of the total organic solids have the composition of urea and about 85% has approximately the same CHO as $C_6H_{12}O_6$. Following the formulas earlier, this leads to

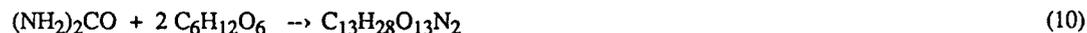


Table 1 shows that the CHON distribution of $C_{13}H_{28}O_{13}N_2$ closely reproduces the reference values.

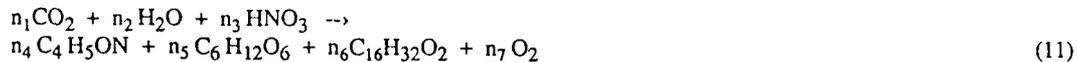
The Waste Processor

The waste processor will receive the both inedible and edible waste plant materials and the human wastes. It will need to handle the edible parts of the plants, for example, if the food supply is too high or is diseased and needs to be scrapped, then material sent to the waste processor will contain some food components. The equations for these processes are essentially various reverse combinations of those above, whereby solids are taken back to CO_2 , H_2O , and HNO_3 . These will not be repeated here. We assume in the model /1/ that this recycling can be accomplished completely using whatever equipment is necessary, although this need not be a requirement in the future, as the output of actual waste processing tests will be added to the model.

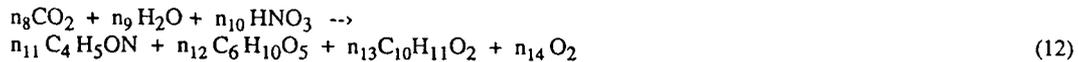
THE SYSTEM

Equations. We now create a system by selective sums of the previously developed equations to form simple balanced transformations for the growth of food and inedible parts by plants, the consumption and respiration of food by humans with the production of wastes, and the recycling back to inorganic forms of all constituents by the waste processor. Specifically, an equation for food production is formed by summing equations (1), (4), and (5). By similarly summing equations (1), (4), (6), and (7) a system for the inedible plant production is obtained. This neglects fats and simple sugars, which are not included here in order to focus on the fiber and lignin components that characterize the inedible portions. The human food equation comes from combining equations (8), (9), and (10) with the reverse of equations (1) and (5). Waste processing the edible parts of plants is the reverse of the growth of food, in other words, summing the reverse of equations (1), (4), and (5); waste processing of the inedible parts is similarly obtained by summing the reverse of equations (1), (4), (6), and (7). Finally, the processing of human waste comes from combining the reverse of equations (1), (4), (5), (8), (9), and (10). These actions lead to the following system:

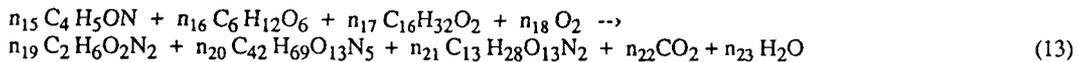
Growth of edible plant matter:



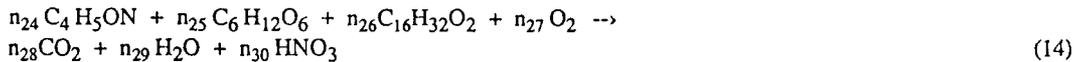
Growth of inedible plant matter:



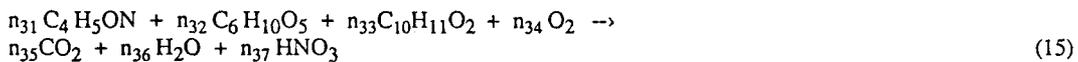
Human metabolism of edible plant matter:



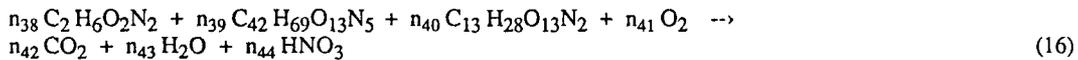
Waste processing of edible plant matter:



Waste processing of inedible plant matter:



Waste processing of human waste:



Equations (11-16) constitute a system for a biological life support system model if the rate coefficients, n_i in moles per unit time, are known.

A Solution

Equations (11-16) must be individually balanced in order that they operate to change matter between various forms and ensure conservation of species. The 44 unknown rate coefficients, n_i ($i = 1 \dots 40$), are not all independent. For example, since N appears in only one component on each side of equations (11), (12), (14), and (15), $n_3 = n_4$, $n_{10} = n_{11}$, $n_{24} = n_{30}$, and $n_{31} = n_{37}$. As another example, since C appears in one constituent on the left-hand side and in three constituents on the right-hand side of equation (11), $n_1 = 4 n_4 + 6 n_5 + 16 n_6$; similar examples are straightforward. Using this procedure for elemental mass balances, 4 equations can be written for each of equations (11-16), resulting in 24 equations for 44 unknowns. Other constraints must be imposed.

The system is therefore further simplified by specifying constant proportionalities between components in physically-meaningful groupings. For example, as the edible part of the wheat grows, the protein, carbohydrate, and fat components are assumed to remain in a constant set of mass ratios to each other. Similarly with the protein, fiber, and lignin in the inedible portion. Furthermore, the edible and inedible are assumed to develop in constant proportion to each other, which means that the harvest index /22/ fraction of edible-biomass/total-biomass acts as a constant governing proportionality during growth (after a 7 day initial period during which only the inedible grows, see /1/). Also, the protein, carbohydrate, and fat in the food consumed are in the same mass proportions as produced by the plant; the masses of urine, feces, and wash solids maintain constant ratios; the waste processor operates upon the protein, carbohydrate, and fat in the edible and the protein, fiber, and lignin in the inedible in the same proportions as they are produced by the plant, and upon the human waste solids in the same relative proportions as they are produced by the people.

With these assumptions it is possible to satisfy the system of reactions by specifying the above proportionalities and by knowing the plant growth rate, the harvest index, the rate of human food consumption, rates of waste processing of edible matter, inedible matter, and human waste. Objections could be raised to all of these assumptions; for example, the amount of protein in the inedible part of wheat decreases as field wheat develops from grass to hay /11/. But they allow us to begin exploring the dynamics of a BLSS model knowing that an approximately equal level of concern exists in specifying the composition of components. More feedbacks can be added as the model develops.

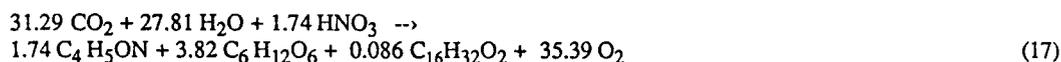
The dynamics of the full model are given in /1/. At this point we will conclude by looking at the system in steady-state. We specify a diet of 855 gm-wheat/day-person, approximately 3000 kcal/day-person /22/. A harvest index of edible to total mass at time of harvest is taken as 45% from a recent experiment /23/. Other trials have had lower harvest indexes /22/, but the 45% is typical of field wheat. The mass proportions of the edible wheat berry are taken as 16.9% protein, 80.5% carbohydrate, and 2.6% fat from Bugbee and Salisbury /22/ (excluding the 2.6% fiber and 2% ash from their total and re-normalizing the values). These proportions are consistent with other values for the wheat grain /13, 24/.

The composition of the inedible portion is more problematical. We choose here a mix of 35% protein, 50% fiber, and 15% lignin. One analysis of wheat straw has close to 30% lignin with the remainder as fiber /25/. Cereal grass of wheat when 10 cm high has a protein content of 43% and even a significant lipid content of 7% /11/. These protein values are partially maintained up to maturity in the hydroponic experiments /26/, although there is some senescence in the later stages of development towards harvest. The fact that the laboratory wheat is not nitrogen-stressed in the later stages of its growth is the likely reason for higher protein fractions in the inedible parts than found under field conditions. Therefore our inedible values should be considered very tentative. When more biochemical dynamics are added to the model, the effects of various environmental factors on the cycling of elements in the total system can be explored by changing the harvest index and inedible composition.

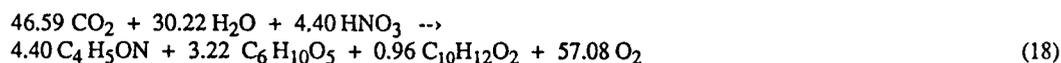
These values lead to 1.74 moles-N in protein consumed per person per day, which in a steady-state must be excreted in the urine, feces, and sweat solids. We distribute this such that $n_{19} = 0.55$, $n_{20} = 0.12$, and $n_{21} = 0.02$ in equation (13). This produces a total urine organic solids of 49.5 gm/day-person, a value generally consistent with a measured value /27/ of total solids of 62.9 gm/day, after subtracting possible values for the percent ash content of total urine solids, 14% /19/, 35% /12/, and 38.2% /16/. The amount of wash organic solids that results from this division is 8.4 gm/day-person, consistent with the 8.8 gm/day-person /16/ after the inorganics and soap are removed from this reference's values. Thus 102.2 gm/day-person is in feces solids, which is substantially higher than the 35.7 gm/day-person found in a 90-day test with highly-processed and easily-digestible foods including meat /27/, but compares better to the 75 gm/day-person for a vegetarian diet /28/.

Using these values, it is possible to compute the molar daily rates for equations (11-16) for a single person. Since the system is in a steady-state, the human eats exactly what the plant consumes, so equation (14) drops away. The results, shown with significant figures that balance the elements to about 0.1%, are as follows:

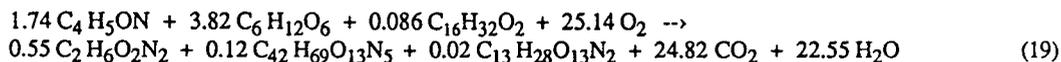
Growth of edible plant matter:



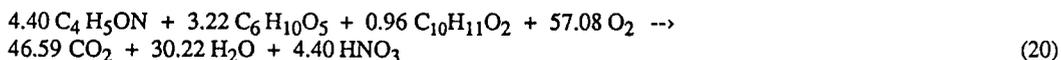
Growth of inedible plant matter:



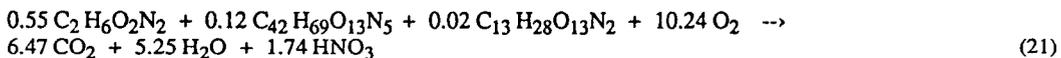
Human metabolism of edible plant matter:



Waste processing of inedible plant matter:



Waste processing of human waste:



CONCLUSION

The whole-system model /1/ lumps some of the components into large-scale masses while maintaining accounting of the CHON elemental balances: food, plant waste, human waste, as well as CO_2 , O_2 , H_2O , and HNO_3 . The flows of these seven mass-types in the steady-state of equations (17-21) is shown in Table 2. Although an alternative would have been to begin directly with a similar set of mass-types values from the literature and estimate a balance of CHON within this system, there would not have been any internal biochemical consistency in such an approach. It is desirable for a system of mass balances to be readily capable of expansion to include, for example, changes in the edible/inedible ratio and tissue-type during growth, the incorporation of different food plants in conjunction with wheat, such as potatoes, soybeans, and lettuce, and the addition of waste processing components that will deal separately with various parts of the inedible biomass, such as lignin and cellulose, which may be important since a substantial portion of the biomass directly from the plant will be indigestible by humans /29/. By explicitly developing a stoichiometric system and examining reasons behind the composition of mass-types, we have a methodology that can adapt to many of these foreseeable needs.

ACKNOWLEDGEMENTS

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TABLE 1 Canonical Formulas and CHON % Composition of Model Constituents

Type and Components	Symbol	C	H	O	N	References and Notes
<u>Edible plant</u>						
Protein	C ₄ H ₅ ON	57.8	6.0	19.3	16.9	C ₄ H ₇ O ₂ N minus peptide bond C ₄ H ₇ O ₂ N mass av.'d amino acid /13/ no. av'd amino acid /13/
		47.5	6.9	31.7	13.9	
		47.0	7.5	30.4	15.1	
		48.3	8.0	28.6	15.1	
Carbohydrate	C ₆ H ₁₂ O ₆	40.0	6.7	53.3	-	assume hexose
Fat	C ₁₆ H ₃₂ O ₂	75.0	12.5	12.5	-	palmitic (C ₁₅ H ₃₁ COOH)
<u>Inedible plant</u>						
Protein	C ₄ H ₅ ON	57.8	6.0	19.3	16.9	see above
Fiber	C ₆ H ₁₀ O ₅	44.4	6.2	49.4	-	represented by cellulose
Lignin	C ₁₀ H ₁₁ O ₂	73.6	6.7	19.6	-	typical formula /11/
<u>Human waste</u>						
Urine solids	C ₂ H ₆ O ₂ N ₂	26.7	6.7	35.6	31.0	(NH ₂) ₂ CO+CH ₂ O /17/ /19/, O by difference p. 840 of /12/ urea: (NH ₂) ₂ CO
		27.8	6.1	33.3	32.8	
		20.9	5.8	47.5	25.8	
		21.3	7.1	26.2	45.5	
		20.0	6.7	26.7	46.7	
Feces solids	C ₄₂ H ₆₉ O ₁₃ N ₅	59.2	8.1	24.4	8.2	2:1:1; protein, fat, hexose Table 3-1 of /16/ /19/, O by difference
		71.1	4.2	12.3	12.3	
		46.5	7.3	37.0	9.2	
Wash solids	C ₁₃ H ₂₈ O ₁₃ N ₂	37.1	6.7	49.5	6.7	15%urea, 85%hexose orgs without soap /16/ orgs including soap /16/
		40.3	6.3	46.8	6.6	
		54.2	7.9	33.2	4.7	

TABLE 2 Mass Fluxes* for a Steady-State System with Wheat as Food

Mass Type	Plants		Human		Waste Processor	
	In	Out	In	Out	In	Out
CO ₂	3426.82	-	-	1092.30	-	2334.52
H ₂ O**	1044.56	-	-	405.96	-	638.60
HNO ₃	387.16	-	-	-	-	387.16
O ₂	-	2958.79	804.62	-	2154.17	-
Food	-	855.00	855.00	-	-	-
Plant Waste	-	1044.75	-	-	1044.75	-
Human Waste	-	-	-	161.36	161.36	-

* All values in gm/person-day calculated using integer atomic masses and equations (17-21).

**H₂O values include only that involved in stoichiometric transformations of mass type, which does not include transpiration, drinking water, water associated with wet (as opposed to dry) biomass, etc. See /1/ for these values.

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