TN 2

SUMMARY OF EUROPEAN LIFE SUPPORT SYSTEMS TECHNOLOGIES

MELISSA ADAPTATION FOR SPACE PHASE II

ESTEC/Contract Nº 20104/06/NL/CP

APPROVAL LIST		
NAME	SIGNATURE	DATE
Prepared by: V. Guirado S. Podhajsky		
Revised by: J. Duatis J. Mas		
Approved by: J. Mas		

DISTRIBUTION LIST		
NAME	POSITION	COMPANY
Ch. Lasseur	TEC-MCT	ESTEC

CHANGE RECORD			
AUTHOR	ISSUE	DATE	CHANGE
J. Duatis V. Guirado	1draft	25/06/07	New Document
V. Guirado S. Podhajsky	1.0	28/03/08	Overall design of the document

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

LIST OF ACRONYMS

AG	Atmosphere Generator
ALISSE	Advanced Life Support System Evaluator
ANITA	Analysing Interferometer for Ambient Air
ARES	Air Revitalisation System
AW	Arthrospira Washer
BPU	Biomass Pre-treatment Unit
BR_CI	Bioreactor of Compartment I
BR_CII	Bioreactor of Compartment II
BR_CIII	Bioreactor of Compartment III
BR_CIVa	Bioreactor of Compartment IVa
C	Atomic Carbon
CC	Crew Chamber
CCA	Carbon dioxide Collection Assembly
C_HPC	Condenser of Higher Plants Chamber
CDC	Carbon dioxide Collector
CRA	Carbon dioxide Reduction Assembly
CI	Compartment I
CII	Compartment II
CIII	Compartment III
CIVa	Compartment IVa
CIVb	Compartment IVb
CV	Compartment V
DNA	Deoxyribonucleic Acid
ECLSS	Ecological Closed Life Support System
ES	Electrolyser Stack
FTU	Food Treatment Unit
GD	Gas Distributor
GWTU	Grey Water Treatment Unit
H	Atomic Hydrogen
HPC	Higher Plants Chamber
LCD	Liquid Collector and Distributor
LC	Liquid Collector
LD	Liquid Distributor
LSS	Life Support Systems
MELiSSA	Micro-Ecological Life Support System Alternative
MOC	Molecular Oxygen Collector
MIDASS	Microbial Detection In Air System for Space
N	Atomic Nitrogen
O	Atomic Oxygen
OGA	Oxygen Generator Assembly
P	Atomic Phosphate or Purge
P&ID	Process & Instrumentation Diagram
RNA	Ribonucleic acid
RB	Residual Biomass
S	Atomic Sulphur
SD	Solid Distributor
SLS	Solid Liquid Separator
UP	Union Point
UTU	Urine Treatment Unit
VFA	Volatile Fatty Acids
WMU	Water Management Unit
WTU	Water Treatment Unit

LIST OF ABBREVIATIONS

A	Area (m^2)
c	Molar concentration (mol/m^3)
CY	Crop Yield $(kg)_{dry}/(m^2 s)$
E	Chemical Element, $E \in \{C, H, O, N, S, P\}$
f	Mass Fraction
G	Generation Term (mol/s)
h	Molar Fraction
H	Molar Fraction related with the rest of compounds
k	Dissociation Coefficient
ka	Acidity Constant
ka_1	First acidity constant for a bi-acid compound
ka_2	Second acidity constant for a bi-acid compound
kb	Basic Constant
kp	Partition Coefficient
kw	Ionic product of water
M	Molecular Weight (kg/mol)
$m(CH_4)$	Mass fraction of methane produced by the human body (dry weight)
$m(H_2)$	Mass fraction of hydrogen produced by the human body (dry weight)
$\mathbf{n}_0$	Number of moles of water per cubic metre of water (mol/m^3)
Pr	Pressure (Pa)
Pv	Water Vapour Pressure (Pa)
ppm	parts per million
Q	Volumetric Flow (m^3/s)
Q(H2O)	Volumetric Flow of hygiene water (m^3/s)
R	Gas constant (Pa m^3)/(K mol)
r	Distribution Coefficient
T	**T**emperature (K)
Tm	Maintenance rate
TW	Perspired water $(kg)_{water}/(m^2 s)$
VM	Molar Volume (m^3/mol)
W	Mass Flow (kg/s)
X	Conversion Coefficient
Y	Stoichiometry Coefficient
Z	Molar Flow (mol/s)

LIST OF SYMBOLS

α	Equilibrium Constant
ρ	Density (kg/m^3)
%(H2O)	Distribution percentage of hygiene water
%(rec)	Recover percentage of water

LIST OF SUB INDICES

a	Biomasses of food except the additional food $a \in \{Ap, HPc, food\}$
abs	absorption
air	atmospheric air
Ac	Acetic Acid
Ad	Additional supply
Ap	Biomass of *Arthrospira platensis*
b	Non-eatable biomass $b \in \{Rr, fc, New, HPre\}$
bio	Biomass
BIO	Biomass generated in Compartment I
RB	Residual Biomass
But	Butyric Acid
Cap	Caproic Acid
ch	Carbohydrates
CH4	Methane
Com	comestible
Food	Overall food for the crew
Cond	Condensation
Cre	Creatinine
CC	Crew Chamber
d	destinations of hygienic water $d \in \{WC\_fc, WC\_urine\,clearliness\}$
don	Dissolution
ex	Exopolysaccharides
Ein	Inflow
Eout	Outflow
fc	Faeces
G	Gas stream
Gin	Gas inflow
Gout	Gas outflow
Fib	Fibres
Hyg	Hygiene Water
H2	Hydrogen
H2O	Water
H2O_cond	Condensed Water
H2O_re	Residual Water
H2SO4	Sulphate
H3PO4	Phosphate
HPc	Biomass of Comestible Part of Higher Plants
HPre	Biomass of Non-Comestible Part of Higher Plants
i	Chemical species (compounds) considered $i \in \{Ac, ADN, Ap, ARN, BIO, BRe, But, Cap, ch, CH4, CO2, cre, ex, fc, HNO2, HNO3, H2, H2O, H2SO4, H3PO4, CH4, lip, ND, New, NH3, N2, OS, O2, prot, HPc, HPre, Prop, re, Rr, urea, ureico, Val\}$
Inert	Inert
ing	Ingested food
j	Sub-systems, $j \in \{BR\_CI, BR\_CII, BR\_CIII, BR\_CIVa, HPC, CC\}$ Specifically for CI it is $j \in \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, BR\_CI\}$
L	Liquid Phase

lip	Lipids
lipsat	saturated Lipids
Lin	Liquid Inflow
Lin'	Liquid inflow at equilibrium stage
Lout	Liquid Outflow
Lout'	Liquid outflow at equilibrium stage
m	Basic Organic Macromolecules $m \in \{ch, lip, prot\}$
m_Ap	Organic Macromolecules of *Arthrospira platensis* $m\_Ap \in \{DNA, RNA, ch, ex, lip, prot\}$
m_New:	Macromolecules of *Nitrosomonas europaea* and *Nitrobacter winogradskyi* $m\_New \in \{DNA, RNA, ch, lip, prot\}$
m_HPc	Macromolecules of the edible parts of the higher plants $m\_HPc \in \{ADN, ARN, ch, fib, lip, lipsat, prot\}$
m_Rr:	Macromolecules of *Rhodospirillum rubrum* $m\_Rr \in \{DNA, RNA, ch, lip, prot\}$
n	Number of Crew members
ND	Non-Degradable
Ne	Biomass of *Nitrosomonas europaea*
New	Biomass of *Nitrosomonas europaea* and *Nitrobacter winogradskyi*
NH3	Ammonia
No_rec	Non recovered water
Nw	Biomass of *Nitrobacter winogradskyi*
u	Urine compounds $u \in \{SU, H_2SO_4, H_3PO_4\}$
Urine	Urine
Persp	Perspiration
Pot	potable water
Prop	Propionic Acid
prot	Protein
purge	Purge
r	Limiting compound
re	residue
rec	Recovered water
resp	Respiration
Rr	Biomass of *Rhodospirillum rubrum*
Sat	Saturation
Solute	Solute
Sin	Solid Inflow
Sin'	Solid Inflow at Equilibrium stage
Sout	Solid Outflow
Sout'	Solid Outflow at Equilibrium stage
SU	Solid Urine
urea	Urea
ureico	Ureic Acid
v	Vegetable Species $v \in \{rice, onion, spinach, lettuce, potato, tomato, wheat, soja\}$
Val	Valeric Acid
WC_fc	Faeces Flush Water
WC_urine	Urine Flush Water

0. SCOPE

This document contains a review of the existing European Life Support technologies. The work developed herein is based on the bibliography and/or existing models on the diverse available LSS technologies. Based on that this document focuses on the MELiSSA, ARES, GWTU, and UTU technologies, for which such reference bibliography and/or models have been made available.

These technologies are described in terms of the processes that implement and the input and output flows that allow their interconnection. These descriptions are used to build the corresponding mathematical models in EcosimPro©. This yields a number of components which constitute the core of a LSS library, to be utilised in later stages to simulate and optimise a complete ECLSS for use in a planetary scenario.

Other European LSS elements like ANITA or MIDASS have not been addressed at the same level of detail because they implement instrumentation technologies for air quality control (trace gases levels and microbial contamination, respectively) in a closed life support environment. Although central for air quality monitoring and safety purposes, these instruments are not considered in the modelling activities of the overall LSS.

ALISSE criteria are not included at this level and will be incorporated in the next project stage where detailed implementation issues based on P&ID are to be undertaken.

This Technical Note corresponds to the output of WP 4100, as described in [A6].

1. APPLICABLE AND REFERENCE DOCUMENTS

1.1 Applicable Documents

[A 1] Request for Quotation RFQ/3-11481/05/NL/CP – MELISSA Adaptation for Space - Phase 2, ref.: RES-PTM/CP/cp/2005.915, dated 16/11/05

[A 2] Statement of Work MELiSSA Adaptation for Space – Phase 2, Ref. TEC/MCT/2005/3467/In.CL dated November 4th, 2005, Version 1 (Appendix 1 to RFQ/3-11481/05/NL/CP)

[A 3] Special Conditions of Tender, Appendix 3 to RFQ/3-11481/05/NL/CP

[A 4] ESA Fax Ref. RES-PTM/CP7cp/2006.226, dated 29/03/06

[A 5] Minutes of Meeting ESA-NTE Clarification meeting on MELiSSA Adaptation for Space – Phase 2; no reference, dated 20/04/06

[A 6] MELiSSA Adaptation for Space – Phase 2. Addendum to NTE's proposal NTE-MEL2-OF-001. Ref. NTE-MEL2-OF-002, May 2006.

1.2 Reference Documents

[R 1] "Dynamics and steady state operation of a nitrifying fixed bed biofilm reactor: mathematical model based description" Pérez, J., Poughon, L., Dussap, G., Montesinos, J., Gòdia, F. Process Biochemistry 40 (2005) 2359 – 2369.

[R 2] "A structured Model for Simulation of Cultures of the *Cyanobacterium Spirulina platensis* in photobioreactors: I. Coupling between light transfer and growth kinetics" Cornet, J.F., Dussap, C.G., Dubertet, G. Biotechnology and Bioengineering, Vol. 40, Pp 817-825 (1992)

[R 3] MELiSSA Yearly Report for 2004 Activity. Memorandum of Understanding TOS-MCT/2002/3161/In/CL. Vieira da Silva, L., Lasseur, Ch. ESA-EWP 2287 (June 2005)

[R 4] Ordóñez et al. "MELiSSA Higher Plants Compartment modelling using EcosimPro" ICES 004-01-2351 (2004)

[R 5] Favreau, M. et al. "Application of rectangular hyperbola to the lettuce and beet crops". ICES 2005-01-2823 (2005)

[R 6] CDF Study Report. Human Spaceflight Vision. European Man-tended Moon Base. CDF-23(A). (2004)

[R 7] CDF Study Report. Architecture Study for Sustainable Lunar Exploration. CDF-33(A). December 2004

[R 8] Drysdale, A.E., Lunar Bioregenerative Life Support Modeling, SAE Technical Paper Series No. 941456 (1994)

[R 9] Levri, J.A. et al. Advanced Life Support Equivalent System Mass Guidelines Document. NASA TM-2003-212278 (2003)

[R 10] Advanced Life Support Baseline Values and Assumptions Document. Hanford, A.J. et al. (2004). NASA JSC-47804

[R 11] Hanford, A.J. Advanced Life Support Research and Technology. Development Metric – Fiscal Year 2004. NASA CR-2004-208944. (October 2004)

[R 12] Hanford, A.J. Advanced Life Support Systems Integration, Modelling and Analysis Reference Mission Document. NASA JSC-39502 (2001)

[R 13] Fulgent N., Poughon L., Richalet J., Lasseur C. Melissa, global control strategy of the artificial ecosystem by using first principles models of the compartments. Advances in Space research (1999), 24(3), 397-405.

[R 14] MELiSSA Memorandum of Understanding, Contract No. 19071/05/NL/CP

[R 15] Mas, J. L. et al., "Design Approach of Closed Loop Food Systems in Space", ICES 2005-01-2920 (2005)

[R 16] Vanrobaeys, X. et al., "A Crop Selection Algorithm for Closed Loop Food Systems" ICES 2005-01-2817, (2005)

[R 17] Proposal in response to ESA RFQ/3-11481/05/NL/CP MELiSSA Adaptation for Space - Phase 2, Ref. NTE-MEL2-OF-001, issue 1, 25/01/05

[R 18] Albiol, J. et al. Preliminary Review of the Pilot plant Final Loop; MELiSSA Technical note 47.3, December 2000

[R 19] Lasseur, Ch. Et al. MELiSSA: Overview of the Project and Perspectives, ICES 2005-01-3066, (2005)

[R 20] Schrunk, D. et al. The Moon: Resources, Future Development and Colonization. John Wiley & Sons – Praxis Publishing Ltd. 1999

[R 21] Eckart, P., The Lunar Base Handbook, Chapter 16, The McGraw-Hill Companies, 1999

[R 22] ECSS-E-30 Part 4A: Environmental Control and Life Support, 5 August, 2005

[R 23] Advanced Life Support Requirements Document, NASA document CTSD-ADV-245C, February 2003

[R 24] ALS Baseline Values and Assumptions Document, JSC-47804, NASA CTSD-ADV-484A, August 2004

[R 25] Microgravity Research in Support of Technologies for the Human Exploration and Development of Space and Planetary Bodies. Commission on Physical sciences, Mathematics and Applications. National Research Council. International Standard Book Number 0-309-06491-0. National Academy Press, 2000

[R 26] ST9-4000-TN-021-NTE, issue 1.1, 28/05/05, Technical Note 3: Model Simulation and Trade-off, Closed Loop Food Systems ST9.1

[R 27] NASA-SRD-3000. Man-Systems Integration Standards. Revision B, July 1995

[R 28] Ch. Lasseur, C. Paille. MELiSSA 2000 Final Report. Memorandum of Understanding. ECT/FG/MMM/97.012. ESA/EWP-2168, September 2001

[R 29] J. Brunet, JJ. Leclercq, O. Gerbi. - Overall Simulator for Life Support Strategy. Technical note TN3. SHERPA P1275 engineering, 11-12-2006

[R 30] J. Rodríguez. Modelling Anaerobic Mixed Cultura Fermentations. Universidad de Santiago de Compostela. June 2006

[R 31] L. Vieira da Silva, Ch. Lasseur. MELiSSA 2004 Final Report. Memorandum of Understanding.TOS-MCT/2002/3161/In/CL. ESA/EWP-2287

[R 32] Anonymous (1997). What is the composition of urine, Sciencenet. 2002

[R 33] ESA Water Quality Standards in manned space vehicles, ref.: ESA-PSS-03-402, issue 1, October 1994

[R 34] Grey Water Recycling Unit Technical Note 2.2. Preliminary Design of the Grey Water Treatment Unit, ref.: TM/GWRU.TN2.2/06.07/JCL, Technomembranes Dévelopment, June 2007

[R 35] MELiSSA Loop Mass Balance Modelling with Matlab®/Simulink. Technical Note 79.2, Issue 1.0 draft, Université Blaise Pascal-LGCB

[R 36] L. Poughon, et al., MELiSSA Loop: First Estimate of Flow Rates and Concentrations through the Loop. ICES Paper 2000-01-2380.

[R 37] Brunet J., Gerbi O., Leclercq JJ. Definition of technical requirements on the simulator. SHERPA, July 2005. 18878/05/NL/CP

[R 38] http://ecls.esa.int/ecls/?p=melissacompartments3

[R 39] Elvira J., MELiSSA TN 72.1, Review of the Complete MELiSSA Loop and Identification of the Critical developments. ESTEC/CONTRACT: 15671/01/NL/ND, July 2002.

[R 40] Stuffler, T. et al., The Air Quality Monitor ANITA – Going into Operation on the International Space Station. ICES Paper 2007-01-3148.

2. INTRODUCTION

2.1 Background

Latest developments in the international Space community have shown a rising interest on the human exploration of the outer space, notably setting objectives of manned missions to Mars by 2030. The return to the Moon seems to be a logical intermediate step in order to test overall mission approach and technology readiness.

In addition, the Moon itself offers other elements of interest that might justify the settlement of a lunar base with a long-term human presence (e.g. exploration or scientific purpose like Planetary Science or Astronomical laboratories, exploitation of local resources etc.).

Whatever the purpose of such lunar base may be, a Life Support System (LSS) specifically designed to sustain the crew over a prolonged period of time is required. Such LSS will need to possess a high degree of closure in order to ensure the maximum level of recycling and minimising the re-supply needs. This fact leads to the consideration of bio-regenerative technologies for the LSS implementation.

2.2 Objective

In the context of manned lunar exploration it is assumed that a Moon base and its associated infrastructure will be in place on the lunar surface to sustain the human presence. The objective of the study is to evaluate the feasibility of progressively assembling an integrated closed-loop Life Support System in a dedicated European module within the Moon base and to operate it with the metabolic products and needs of the crew for demonstration purposes. The basic life support functionalities need to be fulfilled:

- Air revitalization,
- Food production,
- Waste management and
- Water recycling.

The performance requirements demanded for this closed loop Life Support System, assuming a 4-member crew, are:

- The air shall be recycled to close to 100%
- The water shall be recycled to >90%
- Up to 5% of the food for the crew of four shall be produced in a first phase, then up to 40% as final performance

It is envisaged to assemble the closed loop Life Support System units in a suitable sequence to allow for closing all the life support system flows in an efficient manner so that the final performance requirements can be attained progressively. MELiSSA shall be the baseline technology of this closed-loop LSS, complemented with other European LSS technologies like ARES, UTU or GWTU.

Chapter 3 describes all the MELiSSA compartments and the equations that connect the respective inputs and outputs. It also describes additional elements that will be needed in a later stage for the implementation of the model. Chapters 4, 5 and 6 address the ARES, UTU and GWTU technologies, respectively, in similar terms. This baseline work has been used for the implementation of an European EcosimPro® LSS library, described in the Appendix. This library will be used in later stages of the project for modelling, analysing and dimensioning the MELiSSA-based LSS.

3. MELISSA

It is useful to perform a qualitative analysis in order to gain in-depth knowledge on each process of MELiSSA. As it is a biological system, there is a constant biomass production, which contains the elements, E, of the system (C, H, O, N, S, P). This required an analysis of the biomass flow, which has to be separated from the liquid phase.

3.1 The Chemical Compounds in MELiSSA

The micro-organism's and higher plant's biomass, as well as the food's biomass, is composed basically by the elements:

- Carbon (C)
- Hydrogen (H)
- Oxygen (O)
- Nitrogen (N)
- Sulphur (S)
- Phosphor (P).

Therefore, each compound in MELiSSA is a substance composed of these elements. However, it shall be noted that in the mathematic model salts, like Na^+, K^+, Ca^+, Mg^{2+}, Cl^-, as well as heavy metals like Ni, Ag, Zn and Cu, and hormones have not been taken into account due to their irrelevance for these calculations. However, these compounds are very important and a strict study should be done to quantify their flows in each subsystem in the future. Meanwhile a qualitative summary about the flow of salts, heavy metals and hormones is presented in section 3.3.

Additionally, there are some acids and/or some bases to maintain the desired pH in the bioreactors. They have not been taken into account in the model and it is assumed that their accumulation is inhibited by the purges.

In Table 3-1 the sub-indices of the equations used to represent the chemical compounds are shown. Furthermore, the components flowing through the MELiSSA loop are shown in Table 3-2.

Sub-index	Compound
Ac	Acetic Acid
Ap	Biomass of *Arthrospira platensis*
BIO	Biomass of Microorganisms in C I
But	Butyric Acid
Cap	Caproic Acid
ch	Carbohydrates
CH4	Methane
cre	Creatinine
DNA	Deoxyribonucleic Acid
ex	Exopolysaccharides
fc	Faeces
HNO2	Nitrite
HNO3	Nitrate
HPc	Biomass of Eatable Part of Plants
HPre	Residual Biomass of Plants
H2	Hydrogen
H2O	Water

H2SO4	Sulphate
Sub-index	Compound
H3PO4	Phosphate
lip	Lipids
New	Biomass of *Nitrosomonas europaea* and *Nitrobacter winogradskyi*
NH3	Ammoniac
N2	Nitrogen
O2	Oxygen
Prop	Propionic Acid
prot	Proteins
RB	Residual Biomass
re	Residual Organic Matter
RNA	Ribonucleic Acid
Rr	Biomass of *Rhodospirillum rubrum*
SU	Solid Urine
urea	Urea
ureic	Ureic acid
urine	Urine
Val	Valeric Acids

Table 3-1: Compounds from MELiSSA

Sub-index	Compound
Ac	Acetic Acid
Ap	Biomass of *Arthrospira platensis*
But	Butyric Acid
Cap	Caproic Acid
CH4	Methane
cre	Creatinine
fc	Faeces
HNO3	Nitrate
HPc	Biomass of Eatable Part of Plants
HPre	Residual Biomass of Plants
H2	Hydrogen
H2O	Water
H2SO4	Sulphate
H3PO4	Phosphate
New	Biomass *Nitrosomonas europaea* y *Nitrobacter winogradskyi*
NH3	Ammoniac
N2	Nitrogen
Prop	Propionic Acid
RB	Residual Biomass
Rr	Biomass of *Rhodospirillum rubrum*
urea	Urea
ureic	Ureic acid
Val	Valeric Acids

Table 3-2: Compounds that can flow through MELiSSA loop

3.2 Biomass Flow

The processes that take place in each compartment are summarized in Figure 3-1. Assuming that the MELiSSA loop is able to produce approximately 40% of the crew's food intake, the

system must have at least one additional food input for the remaining 60%. Consequently, at least one output is required.

Chemical Reactions

Compartment I

RESIDUAL BIOMASS→ VFA + CO_2 + NH_3 + H_2 + H_2SO_4+ H_3PO_4 + INERT + BIOMASS_1

Compartment II

VFA + NH_3 + H_2SO_4 + H_3PO_4 → BIOMASS_2 (*R. rubrum*) + CO_2 + H_2O

Compartment III

O_2 + CO_2 + NH_3 + H_2SO_4 + H_3PO_4 → BIOMASS_3 (*Nitrosomonas and Nitrobacters*) + HNO_3 + H_2O

Compartment IVa

HNO_3 + H_2SO_4 + H_3PO_4 + CO_2 → BIOMASS_4a (*A. platensis*) + O_2 + H_2O

Compartment IVb

HNO_3 + H_2SO_4 + H_3PO_4 + HNO_3 + NH_3 + CO_2 + H_2O → BIOMASS_4b (Higher plants) + O_2

Compartment V

FOOD + O_2 + WATER → FAECES + URINE + CO_2 + H_2O

Process without Chemical Reaction

Biomass residual generation

BIOMASS_2 + BIOMASS_3 + BIOMASS_4b_non-eatable + FAECES → RESIDUAL BIOMASS

Higher Plant Biomass Separation

BIOMASS_4b → BIOMASS_4_b_eatable + BIOMASS_4_b_non-eatable

Food Generation

BIOMASS_4b_eatable + BIOMASS_4a + FOOD → FOOD

Figure 3-1: General processes of MELiSSA

A schematic of the biomass flow within the MELiSSA system is shown in Figure 3-2. The major biomass circulations are:

1. Compartment I (CI) is fed with the biomass accumulated in the residual biomass mixer (RBM), which accumulates the produced biomass from:
   - Compartment II (CII), that consists of the bacteria *R.rubrum*
   - Compartment III (CIII), that consists of the non edible part of the higher plants and the faeces generated by the crew
   - Compartment IV, that consists of an algae compartment and a higher plants compartment which both produce food and non comestible biomass
   - Compartment V (CV), the crew compartment, which generates feaces and urine

2. Approximately 5% of the produced biomass in Compartment I dies and will be degraded in the same anaerobic process. The amount of the biomass that cannot be degraded exits CI and is not used any further.
3. The food for the crew compartment is a mix of the edible biomass that is produced in the loop (CIVa and IVb) and additional biomass supplied from outside the loop to complement the crew's diet.

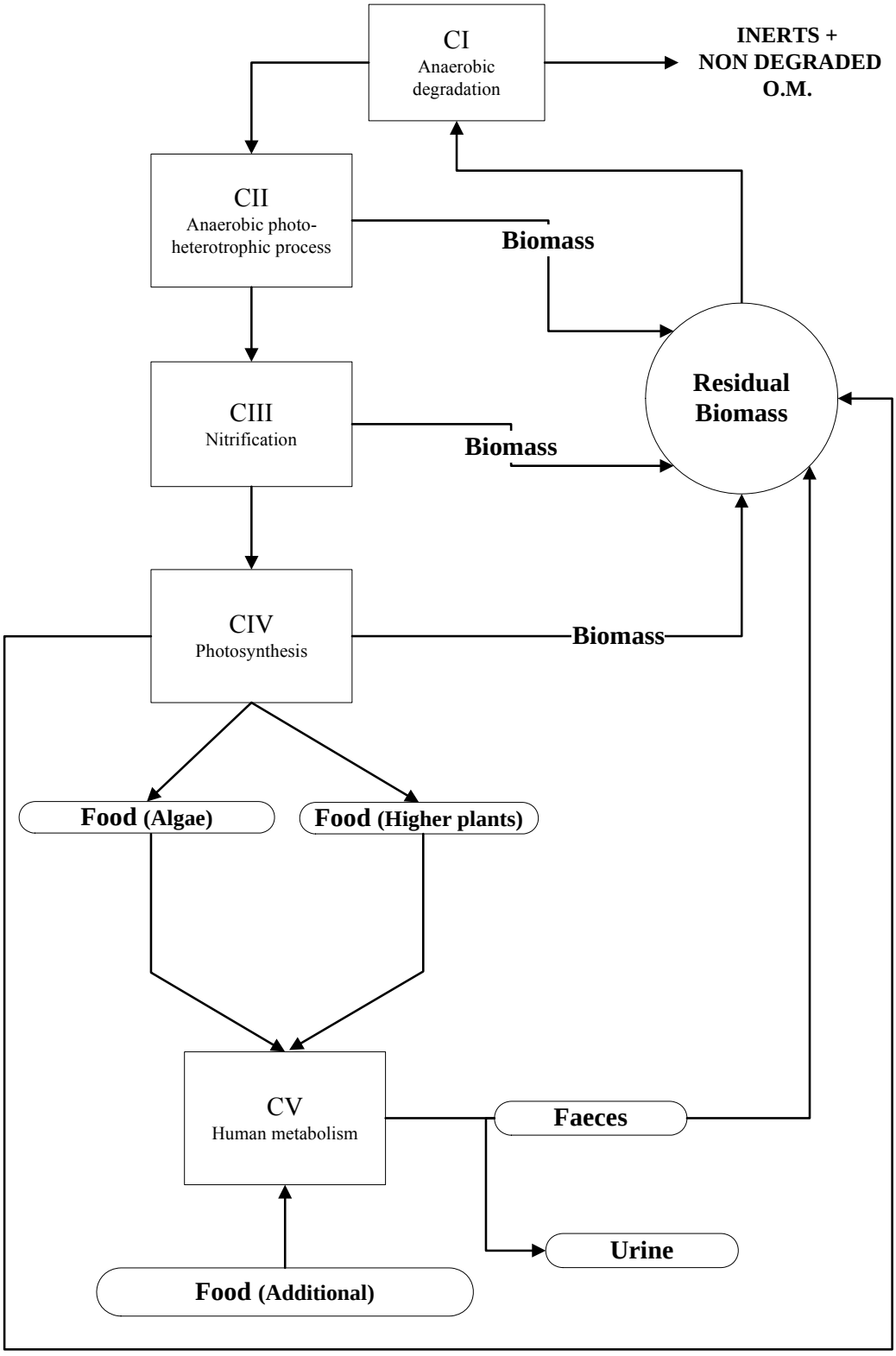


Figure 3-2: Biomass flow

3.3 Salts, Heavy Metals and Hormones flow

As has been explained in the previous section (Figure 3-1), the processes taking place in the MELiSSA loop do not consider salts, heavy metals and hormones, because they do not participate in the reactions. However, the concentrations vary along the loop, depending on the interactions among the transporting streams and the processes that take place.

Figure 3-3 shows the flow of these compounds. Salts and small quantities of heavy metals are ingested by the crew through the food. In ideal conditions, it can be assumed that the human body expels all the elements of the salts and heavy metals ingested with faeces and urine. Additionally, hormones are contained within the urine composition.

Faeces are mixed with the biomass produced in the neighbour compartments as well as water to be degraded in CI. The not degraded organic matter as well as a small quantity of salts and metals is sent out of the system. The liquid leaving CI contains the remaining salts and metals dissolved and passes further through CII and CIII and CIV where algae and higher plants fix certain quantity. The amount not fixed is re-circulated.

Urine, together with its containing salts, metals and hormones is expelled from MELiSSA, but it can be treated through others technologies.

To avoid accumulation, the loop needs several purges, which are not shown in Figure 3-3. The blue colour represents the flow of these substances dissolved in water. The brown colour represents the flow of these substances contained in biomass composition. The orange colour represents the flow of these substances in both forms dissolved and contained in biomass.

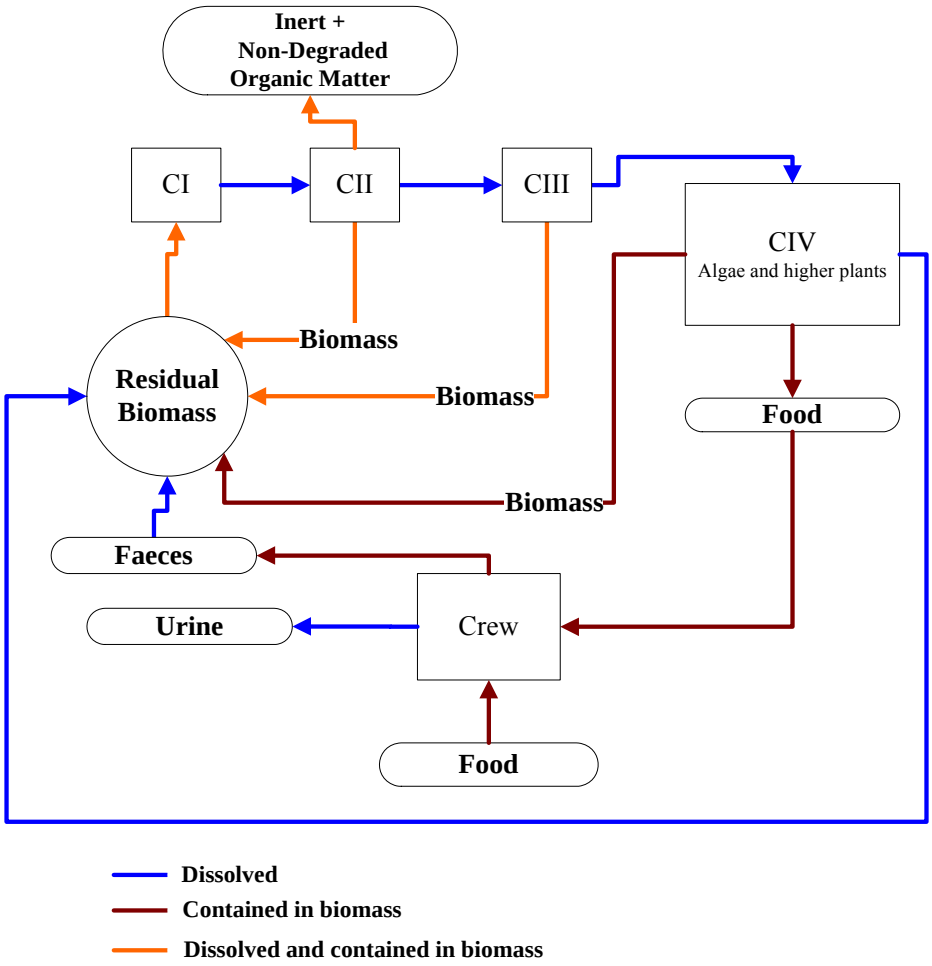


Figure 3-3: Flow of Salts, Heavy metals and Hormones, without display of purges

3.4 General Assumptions

The information available on the various bioreactors of the MELiSSA loop has been exhaustively reviewed. From these sources a mathematical model has been derived and implemented in EcosimPro ®.

A generic mathematic model corresponding to a reference bioreactor has been created without considering kinetic rates and under the assumption that the system works in a steady state, i.e. there is no accumulation. Each process has been characterized by mass balances and partition coefficients enabling the calculation of the distribution of compounds between gas and liquid phases at thermodynamic equilibrium.

Therefore, this mathematic model allows calculating the concentration of each compound "i", in ionic and pure forms in the liquid as well as in pure form in the gas, under the assumptions that the system reaches the equilibrium and that the inputs are known. The model also calculates the gas and liquid volumetric output flows. Thus, by knowing the residence time the system size can be calculated.

The general assumptions in the mathematic model are:

- Each reactor consists of two inputs, Gin (gas) and Lin (liquid), and two outputs, Gout (gas) and Lout (liquid), except for CI.
- The reactor works as a stirred tank and works at atmospheric pressure
- Gas and liquid are in equilibrium when they exit the reactor and their concentrations are related by the Henry constant except for compartments IVb and V where the separation between gas and liquid is done by water transpiration.
- The system works in steady state, thus the accumulation term is zero.
- The kinetic model is not used. Therefore, the generation term is defined by the experimental conversion (regarding a specific reactant).
- The gas behaves as an ideal gas.
- The density of the liquid inflow remains constant.
- The biomass, faeces, higher plants and urine density of the organic matter are considered equal to the water.
- The compounds flowing through the loop are: H_2, O_2, N_2, CO_2, H_2O, NH_3, VFA (acetic, propionic, butyric, valeric and caproic), H_3PO_4, H_2SO_4, HNO_3, and biomass.
- The biphasic compounds are: H_2, O_2, N_2, CO_2, H_2O, NH_3, acetic acid, propionic acid, butyric acid, valeric acid and caproic acid.
- The compounds with ionic form are :
    - Basic compounds: NH_3, H_2O
    - Acid compounds: VFA, H_2O
    - Bi-acid compounds: CO_2

3.5 Additional MELiSSA Subsystems

The MELiSSA concept conceived as closed loop life support system needs some additional units:

- The edible biomass produced in MELiSSA is based on higher plants and algae and it might not supply an equilibrated diet to the crew. Therefore, an additional food supply source is likely to be needed.
- The current anaerobic degradation of Compartment I is circa 70% [RD 38], so that the system needs an output to expel the non-degraded organic matter.
- Purges are needed for the removal of accumulated material that is not converted in the bioreactors.
- Mixers, separators and connectors are needed in order to connect the different flows inside the MELiSSA loop.

Consequently, complementary units, also referred as additional MELiSSA subsystems, need to be modelled to enable a connection between the various MELiSSA compartments. Thus, some units represent connections of streams from different compartments. Other units have the function to diverge non-recycled elements as well as to converge necessary elements from outside the loop. For both options the assumption of a steady state system is made.

Table 3-3 lists the subsystems of the MELiSSA compartments as well as the complementary units. In the followings sections, each subsystem is described and defined through a mathematic model.

Set	Subsystem	Symbol
Compartment I	Bioreactor	BR_CI
	Solid-Liquid Separator	SLS_CI
	Biomass Pre-treatment Unit	BPU
Compartment II	Bioreactor	BR_CII
	Solid-Liquid Separator	SLS_CII
Compartment III	Bioreactor	BR_CIII
	Solid-Liquid Separator	SLS_CIII
Compartment IVa	Bioreactor	BR_CIVa
	Solid-Liquid Separator	SLS_CIVa
Compartment IVb	High Plants Chamber	HPC
	Condenser	C_HPC
Compartment V	Crew Chamber	CC
Collector	Carbone Dioxide Collector	CDC
	Molecular Oxygen Collector	MOC
	Liquid Collector	LC
	Purge	P
	Union Point	UP
	Liquid Collector and Distributor	LCD
	Arthrospira Washing	AW
	Food Treatment Unit	FTU
	Atmosphere Generator	AG

Table 3-3: MELiSSA subsystems

3.6 MELiSSA Bioreactors Mathematic Model Description

A reference model is shown in Figure 3-4, which can be applied to each bioreactor within the MELiSSA loop. However, the calculation of the generation term is different in each case, since the reactions involved in the various compartments are different.

The generic mathematics are explained hereafter and later applied for the resolution of the stoichiometric coefficients in each MELiSSA compartment.

Figure 3-4 shows the model concept with in- and outflows. To simplify the calculations, the inflows of gas G_{in} and liquid L_{in} merge creating a single input E_{in}. Similarly, there is only one output E_{out} that splits up into two streams, gas G_{out} and liquid L_{out}, according to the thermodynamic equilibrium.

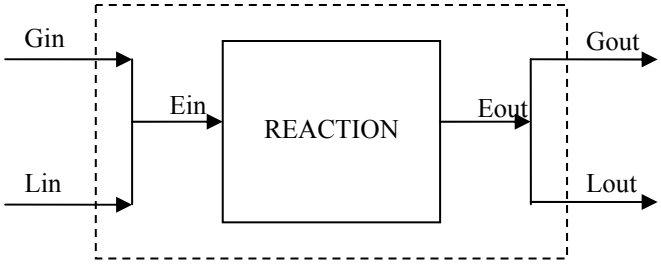


Figure 3-4: Representation of the model

Table 3-4 shows the nomenclature and Table 3-5 shows the data needed for solving the equations.

Symbol	Description	Units
$c_{i,Gin}$	Inlet molar concentration of the compound "i" in the gas stream	mol/m^3
$c_{i,Gout}$	Outlet molar concentration of the compound "i" in the gas stream	mol/m^3
$c_{i,Lin}$	Inlet molar concentration of the compound "i" in the liquid stream	mol/m^3
$c_{i,Lout}$	Outlet molar concentration of the compound "i" in the liquid stream	mol/m^3
$c^{ionic}_{i,Lin}$	Inlet molar concentration of the ionic form of the compound "i" in the liquid stream	mol/m^3
$c^{ionic}_{i,Lout}$	Outlet molar concentration of the ionic form of compound "i" in the liquid stream	mol/m^3
$c^{pure}_{i,Lin}$	Inlet molar concentration of the pure form of compound "i" in the liquid stream	mol/m^3
$c^{pure}_{i,Lout}$	Outlet molar concentration of the pure form of compound "i" in the liquid stream	mol/m^3
G_i	Generation of the compound "i"	mol/m^3
k_i	Coefficient binding the ionic form concentration to the pure form concentration of compound "i" at pressure and temperature of the reactor	-
$k_{a,i}$	Acidity constant of compound "i"(acid compound)	-
$k_{a1,i}$	First acidity constant of compound "i"(bi-acid compound)	-
$k_{a2,i}$	Second acidity constant of compound "i"(bi-acid compound)	-
$k_{b,i}$	Basic constant of compound "i" (base compound)	-
$k_{p,i}$	Partition coefficient of compound "i"	-
k_w	Ionic product of water	-
M_i	Molecular weight of the compound "i"	kg/mol
n_o	Number of mol of water per each litre of water	mol/L
Pr	Pressure in the reactor	Pa
pH	pH conditions inside of the reactor	-
Q_{Gin}	Gas volumetric inflow	m^3/s
Q_{Gout}	Gas volumetric outflow	m^3/s
Q_{Lin}	Liquid volumetric inflow	m^3/s
Q_{Lout}	Liquid volumetric outflow	m^3/s
R	Gas constant	(Pa m^3) / (K mol)
T	Reactor temperature	K
VM	Molar volume at the T and P of the reactor	m^3 /mol
X_r	Conversion referred to a specific compound "r"	-
$Y_{i,j}$	Stoichiometry coefficient where "j" is the type of reaction and "i" is the compound	-
$Z_{i,in}$	Inlet molar flow of the compound "i"	mol/s
$Z_{i,out}$	Outlet molar flow of the compound "i"	mol/s
α_i	Gas-liquid equilibrium constant of compound "i"	-
ρ_G	Density of the gas phase	kg/m^3
ρ_L	Density of the liquid phase	kg/m^3

Table 3-4: Nomenclature

Data	Units
System Specific Data	
Pr	Pa
pH	-
T	K
X_r	-
Composition and Mass Percentages of the Biomass	-
Fixed Data	Units
R	(Pa m^3)/(K mol)
M_i	kg/mol
n_o	mol/m^3
Data used from previous sub-system	Units
$c_{i,Gin}$	mol/m^3
$c_{i,Lout}$	mol/m^3
Q_{Gin}	m^3/s
Q_{Lin}	m^3/s
Variables previously calculated	Units
G_i	mol/s
k_i	mol^{ionic}/mol^{pure}
α_i	$(mol/m^3)_G/(mol/m^3)_L$

Table 3-5: Data

Variables G_i, k_i and α_i, shown in Table 3-5, are not directly known but they can be calculated according to section 3.6.1. These variables are dependent on others, as well as fixed data and subsystem specific data. The fixed data do not vary between the different subsystems. The concentration and the volumetric flows at the inlet are variables depending on the previous subsystem.

The equations of the model can be divided in two groups: general equations and equations for each compound.

General equations:

$$\sum_{i}^{n} c_{i,L1} \cdot M_i = \rho_L \quad (1)$$

$$R \cdot T \cdot \sum_{i}^{n} c_{i,G2} = P \quad (2)$$

$$\sum_{i}^{n} c_{i,Lout} \cdot M_i = \rho_L \quad (3)$$

Equations for each compound, i:

$$0 = Z_{i,Ein} - Z_{i,Eout} + G_i \quad (4)$$

$$Z_{i,Ein} = (Q_{Gout} \cdot c_{i,Gin} + Q_{Lin} \cdot c_{i,Lin}) \quad (5)$$

$$Z_{i,Eout} = (Q_{Gout} \cdot c_{i,Gout} + Q_{Lout} \cdot c_{i,Lout}) \quad (6)$$

$$c_{i,Gout} = c_{i,Lout}^{pure} \cdot \alpha_i \quad (7)$$

$$c_{i,Lout}^{ionic} = c_{i,Lout}^{pure} \cdot k_i \quad (8)$$

$$c_{i,Lout} = c_{i,Lout}^{pure} + c_{i,Lout}^{ionic} \quad (9)$$

$$\text{With } i \in \left\{ \begin{array}{l} Ac, DNA, Ap, RNA, BIO, RB, But, Cap, ch, CH4, CO2, cre, ex, fc, HNO3, \\ H2, H2O, H2SO4, H3PO4, lip, New, NH3, N2, SU, O2, prot, \\ HPc, HPre, Prop, re, Rr, urea, uric, Val \end{array} \right\}$$

As explained, this description is applicable for the bioreactors at compartments I, II, III and IVa. The behaviour of the chambers IVb and V is similar to the bioreactors but the distribution between the gas and liquid phase is different.

3.6.1 Calculation of the Variables: G_i, k_i, α_i

3.6.1.1 Generation Term, G_i

The generation term refers to the quantity of compound "i" that has been consumed (if it is a reactant) or produced (if it is a product). It indicates the number of moles of one reactant with a known conversion coefficient. Thus, knowing the stoichiometric coefficient, the generation of the remaining elements can be calculated, according to equation 10 and 11:

$$G_{i,j} = -Z_{r,Ein} \cdot X_r \cdot \frac{Y_{i,j}}{Y_{r,j}} \quad (10)$$

$$G_i = \sum G_{i,j} \quad (11)$$

→ With $j \in \{BR\_CI, BR\_CII, BR\_CIII, BR\_CIVa, HPC, CC\}$ and for CI $j \in \{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, BR\_CI\}$ with "r" being the specific reactant with the known conversion

→ The equations 10 and 11 are for each compound "i" except for H2O.

Both, the stoichiometric ration, $Y_{i,j}$, and the generation term, $G_{i,j}$, are negative when the substance is a reactant, they are positive when it is a product, or zero if the component is not involved in the reaction.

The calculation to the solution of the generation term is explained in more details for each compartment in sections 3.6.2 through 3.6.5.

3.6.1.2 Dissociation Constant, k_i

In the global system some compounds are present in their ionic form due to the acid-base equilibrium. This equilibrium is considered instantaneous, and it is described by means of the dissociation constant, k_i, depending on the conditions of pH and temperature and the characteristics of the compound [R 28]. The global concentration of the liquid phase has to be split into the concentration of ionic forms and the concentration of pure forms of the compounds (see equation 9) which are related to k_i (see equation 8).

For basic compounds (e.g. ammonia), the equilibrium reaction takes the form:

$$BaseOH + H^+ \Leftrightarrow Base^+ + H_2O$$

The equilibrium constant becomes:

$$k_i = \frac{k_{b,i}}{k_w} \cdot 10^{-pH} \quad (12)$$

For acid compounds (such as fatty acids), the equilibrium reaction takes the form:

$$AcH + H_2O \Leftrightarrow Ac^- + H_3O^+$$

The equilibrium constant becomes:

$$k_i = \frac{k_{a,i}}{10^{-pH}} \quad (13)$$

There are some compounds, like carbon dioxide, that can accept either one or two protons. For these compounds (bi-acids) two equilibrium reactions exist:

$$AcH_2 + H_2O \Leftrightarrow AcH^- + H_3O^+$$
$$AcH^- + H_2O \Leftrightarrow Ac^{2-} + H_3O^+$$

The equilibrium constant takes the form:

$$k_i = \frac{k_{a1,i}}{10^{-pH}} \cdot \left(1 + \frac{k_{a2,i}}{10^{-pH}}\right) \quad (14)$$

It has to be taken into account that one mol of water is consumed per mole of carbonate formation.

The basic and acid constants are dependant on the temperature and follow the Antoine equation:

$$Ln(k) = \frac{A}{T} + B \cdot Ln(T) + C \cdot T + D \quad (15)$$

The coefficients A, B, C and D are experimentally obtained.

3.6.1.3 Equilibrium Gas-Liquid Constant, α

Each sub-system is made up of two phases, gas and liquid, and some chemical compounds are contained in both. The gas-liquid equilibrium constant α of equation (7) [R 28] expresses the correlation of the concentrations of the biphasic compounds of the two phases. It is resolved by the use of the partition coefficient, $kp_{,i}$ (equation 16) [R 29].

$$\alpha_i = \frac{kp_i}{VM \cdot n_o} \quad (16)$$

Where:

$$VM = \frac{22{,}4 \cdot T}{273{,}15} \quad (17)$$

kp_i is obtained by the Antoine equation for the vapour pressure, whose coefficients are determined experimentally and are valid within certain ranges of temperatures (equation 18) [R 28].

$$Ln(kp_i) = A - \frac{B}{C + T} \quad (18)$$

3.6.2 Compartment I: Liquefying Reactor

3.6.2.1 Description

The main objective of Compartment I's reactor is to degrade the residual organic matter from the whole system, through an anaerobic process.

The residual biomass is a mix of faeces produced by the crew in compartment V, biomass generated in the Compartments II and III, and non-edible parts of the plants produced in the Higher Plants Chamber (Compartment IVb):

BIOMASS_2 + BIOMASS_3 + BIOMASS_4b_Inedible + FAECES → RESIDUAL BIOMASS

This residual biomass is degraded to volatile fatty acids (VFA), which will be treated in the second compartment and some other components. The output products are: volatile fatty acids (acetic, propionic, butyric, valeric and caproic acids), carbon dioxide, ammonia, hydrogen, mineral salts and inert matter:

$$\text{RESIDUAL BIOMASS} \rightarrow \text{VFA} + CO_2 + NH3 + H_2 + H_2SO_4 + H_3PO_4 + \text{INERT}$$

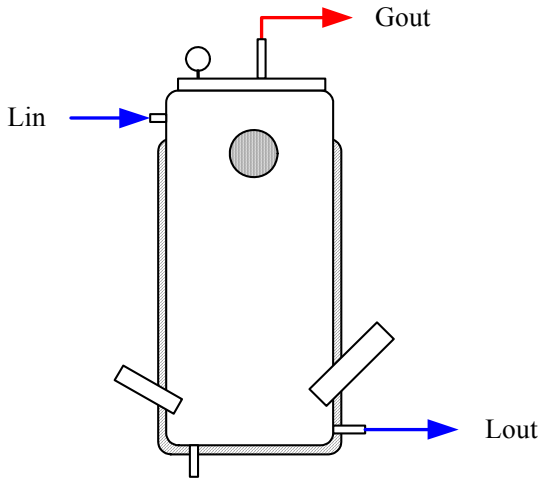


Figure 3-5: Reactor of Compartment I

The in- and out-flows of Compartment I are shown in Figure 3-5. In the latter the concentrations and volume flow rates need to be determined, as well as the amount of non-recycled organic matter and its composition. This results in the following steps:

1. Calculate the molecular weights of macromolecules proteins, carbohydrates and lipids of residual biomass.
2. Calculate the stoichiometry and generation term for each semi-reaction. It also calculates the amount of non-degradable organic matter and the generation term of the overall reaction.
3. Calculate the volume flow rates and concentrations of the reactor output (mass balances and equilibrium)

3.6.2.2 Assumptions

- The methanogenesis is inhibited working at 55ºC and a lightly acid pH
- The generation term is calculated through the experimental conversions of the each bio-molecule and the VFA
- The gas and liquid phases that abandon the bioreactor are in equilibrium

3.6.2.3 Operation Data

Reactor Parameters	Description	Value	Units
Pr	Pressure	101325	Pa
pH	pH conditions	6,7	-
T	Bioreactor Temperature	328	K
R	Ideal Gas Constant	8,31	J/(K mol)

Table 3-6: The reactor parameters and characteristics of CI

Symbol	Description	Value	Units
$f_{H2O,Bio}$	Mass fraction of water in the biomass of the micro-organism that colonize CI	0.5 - 1	-
h_{C_ch}	Molar Fraction of C in the residue that is transformable into C of Carbohydrates	0 - 1	-
h_{N_NH3}	Molar Fraction of N in the residue that is transformable into N of Ammonia	0 - 1	-
h_{S_H2SO4}	Molar Fraction of S in the residue that is transformable into S of H_2SO_4	0 - 1	-
h_{P_H3PO4}	Molar Fraction of P in the residue that is transformable into P of H_3PO_4	0 - 1	-
X_{Ac}	Acetic Acid Conversion; moles of acetic acids that degrade per mole of initial acetic acids	0 - 1	-
X_{Bio}	Biomass conversion; moles of degraded biomass per mole of generated biomass. It is the biomass generated in the own Compartment and not the residual biomass input	0 - 1	-
X_{But}	Butyric Acid Conversion; moles of butyric acids that degrade per mole of initial butyric acids	0 - 1	-
X_{Cap}	Caproic Acid Conversion; moles of caproic acids that degrade per mole of initial caproic acids	0 - 1	-
X_{ch}	Carbohydrate Conversion; moles of carbohydrates that degrade per mole of initial carbohydrate	0 - 1	-
X_{CO2}	Carbon Dioxide Conversion; moles of carbon dioxides that degrade per mole of initial Carbon Dioxide	0 - 1	-
X_{lip}	Lipid Conversion; moles of lipids that degrade per mole of initial lipids	0 - 1	-
X_{prot}	Protein Conversion; moles of proteins that degrade per mole of initial protein	0 - 1	
X_{Prop}	Propionic Acid Conversion; moles of propionic acids that degrade per mole of initial propionic acids	0 - 1	-
X_{Val}	Valeric Acid Conversion; moles of valeric acids that degrade per mole of initial valeric acids	0 - 1	-

Table 3-7: Data production

3.6.2.4 Reactions, Stoichiometry and Generation Term

The liquefying compartment performs anaerobic degradation by a bacterial community that carries out several fermentative conversions. To reduce the complexity of the model only the basic processes and compounds involved are considered. Table 3-8 shows the compounds treated and their elemental composition, as considered in [R 35], with modified proteins' chemistry formula.

Compound	Composition (chemical Formula)					
	C	H	O	N	S	P
Acetic Acid	2	4	2	0	0	0

Ammonia	0	3	0	1	0	0
Butyric Acid	4	8	2	0	0	0
Caproic Acid	6	12	2	0	0	0
Carbohydrates	1	1.6667	0.8333	0	0	0
Carbon Dioxide	1	0	2	0	0	0
Hydrogen	0	2	0	0	0	0
Inert	n	o	p	q	r	s
Lipids	1	1.2	0.125	0	0	0
Microorganism's Biomass of CI	5	7	2	1	0	0
Phosphoric Acid	0	3	4	0	0	1
Propionic Acid	3	6	2	0	0	0
Proteins	1	1.55386	0.28354	0.2681	0	0
Residual Biomass	a	b	c	d	e	f
Residue	g	h	i	j	k	m
Sulfuric Acid	0	2		0	1	0
Varleric Acid	5	10	2	0	0	0
Water	0	2	1	0	0	0

Table 3-8: Elemental composition of the compounds

The composition of each macro molecule may vary with the residual biomass considered. The values in Table 3-8 are assumptions based on average values that are considered to be a good approach for this model.

Phosphorous is an element that can be found in molecules with hydrophilic groups, mainly in composition of lipids, but it can also be found in some proteins and carbohydrates. Sulphur, however, can only be found in some proteins and hardly in the other two substances. The composition of the three bio-molecules given in Table 3-8 is without these two elements, therefore the bio-molecules that contain S and P, have been considered to be in the residue of the residual biomass. When the residue is decomposed, S and P are bound in molecules that are expressed in the calculation as sulphuric and phosphoric acids, respectively.

The processes that have been considered for modelling compartment I are:

1. Disintegration
2. Residue decomposition
3. Carbohydrates hydrolysis
4. Proteins hydrolysis
5. Lipids hydrolysis
6. Propionic oxidation
7. Butyric oxidation
8. Valeric oxidation
9. Caproic oxidation
10. Biomass decays

The stoichiometries of processes 3) to 9) are taken from [R 35] and are fixed. The first step, process 1), serves to calculate the quantity of proteins, carbohydrates, lipids and others (residue) contained in the residual biomass. The procedure applied consists of calculating the generation for each compound in each process. Consequently, the generation term of the anaerobic degradation is the sum of all individual ones.

The processes of methanogenesis that exists normally in a conventional anaerobic degradation will not be taken into account because it is assumed that methane production is inhibited.

The detailed description of each process is provided in the following sections:

A.1 Disintegration

This process is the breakdown of organic matter into residual carbohydrates, proteins, lipids and waste consisting of fibres, DNA, RNA and other biomolecules with sulphur and phosphorus.

$$\left[C_aH_bO_cN_dS_eP_f\right]_{\text{Residual Biomass}}$$

$$\Downarrow$$

$$CH_{1.6667}O_{0.8333} + CH_{1.55386}O_{0.28354}N_{0.2693} + CH_2O_{0.125} + \left[C_gH_hO_iN_jN_kN_m\right]_{\text{Residue}}$$

The chemical formula of the residual biomass (a, b, c, d, e, f), as well as the mass fraction of proteins, carbohydrates and lipids contained in the residual biomass are calculated in the Biomass Pre-treatment Unit (BPU). Therefore, the residue composition (g, h, I, j, k, m) is calculated here.

The molar flow of each macromolecule and of the residue is determined by equations I.1, I.2 and I.3.

$$G_{RB,\,1} = -c_{RB,\,Lin} \cdot Q_{Lin} \qquad \text{(I.1)}$$

$$G_{m,\,1} = -f_{m,RB} \cdot \frac{M_{RB}}{M_m} \cdot G_{RB,\,1} \qquad \text{(I.2)}$$

→ Equation I.2 for each macromolecule “m”, where $m \in \{ch, lip, prot\}$.

$f_{m,\,BRe}$ is the mass fraction of the macromolecule “m”

$$G_{re,\,1} = 1 \qquad \text{(I.3)}$$

With these equations, the residue composition can be fixed, since there are six equations and six unknowns (see Table 3-9 and equation I.4)

Component, i	Generation (mol/s)	Composition					
		C	H	O	N	S	P
Carbohydrates	$G_{ch,\,1}$	1	1.6667	0.8333	0	0	0
Lipids	$G_{lip,\,1}$	1	2	0.125	0	0	0
Proteins	$G_{prot,\,1}$	1	1.55386	0.28354	0.2681	0	0
Residual Biomass	$G_{RB,\,1}$	a	b	c	d	e	f
Residue	1	g	h	i	j	k	m

Table 3-9: Generation and composition of the disintegration process

$$\sum G_{i,1} \cdot E_i = 0 \qquad \text{(I.4)}$$

→ for each element E, where $E \in \{C, H, O, N, S, P\}$. The sum includes each compound "i" from Table 3-9

A.2 Residue Decomposition

The residue consists of fibre, nucleic acids and other substances. The result of the decomposition is ammonia, degradable carbohydrate, sulphates, phosphates and non-degradable inert matter.

$$\left[C_gH_hO_iN_jS_kP_m\right]_{\text{Residue}} \rightarrow CH_{1.6667}O_{0.8333} + NH_3 + H_3PO_4 + H_2SO_4 + \left[C_nH_oO_pN_qS_rP_s\right]_{\text{Inert}}$$

To calculate stoichiometric coefficients it is necessary to know the fraction of C of carbohydrates as well as the fraction of N, S and P of ammonia, sulphuric and phosphoric acids respectively, as described in equation I.5, I.6, I.7 and I.8. Consequently the composition of the inert matter (n, o, p, q, r, s) can be calculated according to equation I.9 and Table 3-10.

Component, i	Stoichiometric Coefficient Y	Composition					
		C	H	O	N	S	P
Carbohydrates	$Y_{ch,2}$	1	1.6667	0.8333	0	0	0
H_2SO_4	$Y_{H2SO4,2}$	0	2	4	0	1	0
H_3PO_4	$Y_{H3PO4,2}$	0	3	4	0	0	1
Inert	1	n	o	p	q	r	s
NH_3	$Y_{NH3,2}$	0	3	0	1	0	0
Residue	-1	g	h	i	j	k	m

Table 3-10: Stoichiometry and composition of the Residue Decomposition

$$Y_{ch,2} = h_{C\_ch} \cdot g \quad \text{(I.5)}$$

$$Y_{NH3,2} = h_{N\_NH3} \cdot j \quad \text{(I.6)}$$

$$Y_{H2SO4,2} = h_{S\_H2SO4} \cdot k \quad \text{(I.7)}$$

$$Y_{H3PO4,2} = h_{P\_H3PO4} \cdot m \quad \text{(I.8)}$$

$$\sum Y_{i,2} \cdot E_i = 0 \quad \text{(I.9)}$$

→ The equation I.9 counts for each element E. The sum includes the components "i" from Table 3-10

Once the stoichiometry equations are expressed and under the assumption of a complete decomposition of the residue, the generation for each component in this process is expressed by equation I.10.

$$G_{i,2} = -G_{re,1} \cdot \frac{Y_{i,2}}{Y_{re,2}} \quad \text{(I.10)}$$

→ it accounts for each compound "i" from Table 3-10 . For the remaining compounds the generation is zero due to the decomposition of the residue (process 2) as the stoichiometric coefficients is zero.

The stoichiometry of the process below (reactions from 3 to 9) is fixed [R35].

A.3 Carbohydrates Hydrolysis & Acidogenesis

$$6.546\,CH_{1.6667}O_{0.8333} + 0.1091\,NH_3 + 0.0968\,H_2O$$

$$\downarrow$$

$$1.3333\,C_3H_6O_2 + 0.6667\,C_2H_4O_2 + 0.6667\,CO_2 + 0.1091\,C_5H_7O_2N$$

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Acetic	0.6667	2	4	2	0	0	1
Biomass	0.1091	5	7	2	1	0	0
Carbohydrates	-6.546	1	1.6667	0.8333	0	0	0
CO_2	0.6667	1	0	2	0	0	0
H_2O	-0.0968	0	2	1	0	0	0
NH_3	-0.1091	0	3	0	0	0	0
Propionic	1.3333	3	6	2	0	1	0

Table 3-11: Stoichiometry and composition of the carbohydrates hydrolysis

$$G_{i,3} = -X_{ch} \cdot (G_{ch,1} + G_{ch,2}) \cdot \frac{Y_{i,3}}{Y_{ch,3}} \qquad \text{(I.11)}$$

→ for each compound "i" from Table 3-11. The generation of the carbohydrates hydrolysis (process 3) of the remaining compounds is zero.

A.4 Proteins Hydrolysis & Acidogenesis

$$CH_{1.55386}O_{0.28354}N_{0.2681} + 0.5440H_2O$$
$$\downarrow$$
$$0.0237\,C_5H_7O_2N + 0.01703\,C_6H_{12}O_2 + 0.0174\,C_5H_{10}O_2 + 0.0187\,C_4H_8O_2 + 0.0601\,C_3H_6O_2$$
$$+ 0.1608\,C_2H_4O_2 + 0.1055\,H_2 + 0.11604\,CO_2 + 0.2444NH_3$$

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Acetic	0.1608	2	4	2	0	0	1
Biomass	0.0237	5	7	2	1	0	0
Butyric	0.0187	4	8	2	0	0	0
Caproic	0.01703	6	12	2	0	0	0
CO_2	0.1164	1	0	2	0	0	0
H_2	0.1055	0	2	0	0	0	0
H_2O	-0.0968	0	2	1	0	0	0
NH_3	0.2444	0	3	0	1	0	0
Propionic	0.0601	3	6	2	0	1	0
Proteins	-1	1	1.55386	0.28354	0.2681	0	0
Valeric	0.0174	5	10	2	0	0	0

Table 3-12*: Stoichiometry and composition of the proteins hydrolysis*

$$G_{i,4} = -X_{prot} \cdot (G_{prot,1}) \cdot \frac{Y_{i,4}}{Y_{CH,4}} \qquad \text{(I.12)}$$

→ for each compounds "i" from Table 3-12. The generation of the protein hydrolysis (process 4) of the remaining compounds is zero.

A.5 Lipids Hydrolysis

$$0.95\,CH_2O_{0.125} + 0.05\,NH_3 + 0.68125\,H_2O \rightarrow 0.05\,C_5H_7O_2N + 0.83125\ H_2 + 0.35\,C_2H_4O_2$$

Compounds, i	Stoichiometric coefficient, Y	Sub index (composition)					
		C	H	O	N	S	P
Acetic	0.35	2	4	2	0	0	1
Biomass	0.05	5	7	2	1	0	0
H2	0.83125	0	2	0	0	0	0
H2O	-0.68125	0	2	1	0	0	0
Lipids	-0.95	1	2	0.125	0	0	0
NH3	-0.05	0	3	0	0	0	0

Table 3-13: Stoichiometry and composition of the lipids hydrolysis

$$G_{i,5} = -X_{lip} \cdot (G_{lip,1}) \cdot \frac{Y_{i,5}}{Y_{lip,5}} \qquad \text{(I.13)}$$

→ for each compound "i" from Table 3-13. The generation of the lipids hydrolysis (process 5) of the remaining compounds is zero.

A.6 Propionic Oxidation

$$C_3H_6O_2 + 0.05\,NH_3 + 1.85\,H_2O \rightarrow 0.875\,C_2H_4O_2 + 3\,H_2 + CO_2 + 0.05\,C_5H_7O_2N$$

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Acetic	0.875	2	4	2	0	0	1
Biomass	0.05	5	7	2	1	0	0
CO_2	1	1	0	2	0	0	0
H_2	3	0	2	0	0	0	0
H_2O	-1.85	0	2	1	0	0	0
NH_3	-0.05	0	3	0	0	0	0
Propionic	-1	3	6	2	0	0	0

Table 3-14: Stoichiometry and composition of the propionic oxidation

$$G_{i,6} = -X_{Prop} \cdot (G_{Prop,3} + G_{Prop,4}) \cdot \frac{Y_{i,6}}{Y_{Prop,6}} \qquad (I.14)$$

→ for each compound "i" from Table 3-14. The generation for the propionic oxidation (process 6) of the remaining compounds is zero.

A.7 Butyric Oxidation

$$C_4H_8O_2 + 0.05\,NH_3 + 1.85\,H_2O \rightarrow 1.875\,C_2H_4O_2 + 2\,H_2 + 0.05\,C_5H_7O_2N$$

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Acetic	1.875	2	4	2	0	0	1
Biomass	0.05	5	7	2	1	0	0
Butyric	-1	4	8	2	0	0	0
H_2	2	0	2	0	0	0	0
H_2O	-1.85	0	2	1	0	0	0
NH_3	-0.05	0	3	0	0	0	0

Table 3-15: Stoichiometry and composition of the butyric oxidation

$$G_{i,7} = -X_{But} \cdot (G_{But,4}) \cdot \frac{Y_{i,7}}{Y_{But,7}} \qquad (I.15)$$

→ for each compound "i" from Table 3-15. The generation for the butyric oxidation (process 7) of the remaining compounds is zero.

A.8 Valeric Oxidation

$$C_5H_{10}O_2 + 0.05\,NH_3 + 3.85\,H_2O \rightarrow 1.875\,C_2H_4O_2 + 5\,H_2 + CO_2 + 0.05\,C_5H_7O_2N$$

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Acetic	1.875	2	4	2	0	0	1
Biomass	0.05	5	7	2	1	0	0
CO_2	1	1	0	2	0	0	0
H_2	5	0	2	0	0	0	0
H_2O	-3.85	0	2	1	0	0	0
NH_3	-0.05	0	3	0	0	0	0
Valeric	-1	5	10	2	0	0	0

Table 3-16: Stoichiometry and composition of the valeric oxidation

$$G_{i,8} = -X_{Val} \cdot (G_{Val,4}) \cdot \frac{Y_{i,8}}{Y_{Val,8}} \qquad \text{(I.16)}$$

→ for each compound "i" from Table 3-16. The generation for the valeric oxidation (process 8) of the remaining compounds is zero.

A.9 Caproic Oxidation

$$C_6H_{12}O_2 + 0.05\,NH_3 + 3.85\,H_2O \rightarrow 2.875\,C_2H_4O_2 + 4\,H_2 + 0.05\,C_5H_7O_2N$$

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Acetic	2.875	2	4	2	0	0	1
Biomass	0.05	5	7	2	1	0	0
Caproic	-1	6	12	2	0	0	0
H_2	4	0	2	0	0	0	0
H_2O	-3.85	0	2	1	0	0	0
NH_3	-0.05	0	3	0	0	0	0

Table 3-17: Stoichiometry and composition of the caproic oxidation

$$G_{i,9} = -X_{Cap} \cdot (G_{Cap,4}) \cdot \frac{Y_{i,9}}{Y_{Cap,9}} \qquad \text{(I.17)}$$

→ for each compound "i" from Table 3-17. The generation for the caproic oxidation (process 9) of the remaining compounds is zero.

A.10 Biomass Decay

This process reflects the death of the micro-organisms that colonize the bioreactor. When they die, their biomass degrades to hydrogen, ammonia and carbon dioxide:

$$C_5H_7O_2N + 8\,H_2O \rightarrow NH_3 + 10\,H_2 + 5\,CO_2$$

In reality, this process is very slow, and the conversion of this reaction, referring to the biomass of microorganisms, X_{BIO}, always will be very small.

Component, i	Stoichiometric Coefficient, Y	Composition					
		C	H	O	N	S	P
Biomass	-1	5	7	2	1	0	0
CO_2	5	1	0	2	0	0	0
H_2	10	0	2	0	0	0	0
H_2O	-8	0	2	1	0	0	0
NH_3	1	0	3	0	1	0	0

Table 3-18: Stoichiometry and composition of the biomass decays process

The generation term is:

$$G_{i,10} = -X_{BIO} \cdot (G_{BIO,3} + G_{BIO,4} + G_{BIO,5} + G_{BIO,6} + G_{BIO,7} + G_{BIO,8} + G_{BIO,9}) \cdot \frac{Y_{i,10}}{Y_{BIO,10}} \qquad \text{(I.18)}$$

→ for each compound "i" from Table 3-18. The generation for the biomass decay (process 10) of the remaining compounds is zero.

Adding up all semi-reactions taking place during anaerobic degradation, the overall reaction takes the form (without stoichiometric coefficients):

$$[C_aH_bO_cN_dS_eP_f]_{\text{Residual Biomass}} + H_2O$$
$$\downarrow$$
$$CH_{1.6667}O_{0.8333} + CH_{1.56828}O_{0.3063}N_{0.2693} + CH_2O_{0.125} + H_2SO_4 + H_3PO_4 + C_2H_4O_2 + C_3H_6O_2 + C_4H_8O_2 + C_5H_{10}O_2 + C_6H_{12}O_2 + CO_2 + H_2 + NH_3 + CH_4 + [C_mH_nO_oN_pS_qP_r]_{\text{Inert}}$$

The global generation term (equation I.19) describes the number of moles of each substance produced in the anaerobic reactor

$$G_{i,BR\_CI} = \sum_j G_{i,j} \qquad \text{(I.19)}$$

→ for each compound "i" except the biomass. The sum covers the generation compound of "i" in each process "j", where $j \in \{1,2,3,4,5,6,7,8,9,10,11,12\}$

In the global reaction proteins ($CH_{1.56828}O_{0.3063}N_{0.2693}$), carbohydrates ($CH_{1.6667}O_{0.8333}$) and lipids ($CH_2O_{0.25}$) that have not been degraded, as well as inert ($C_mH_nO_oN_pS_qP_r$), form the non-degradable residual biomass which, together with the non-degradable anaerobic micro-organism ($C_5H_{10}O_2$), is considered as a new residual biomass (RB). This RB is suspended and exits the system through a Solid-Liquid Separator. Equation I.20 is used to calculate its mass flow, $W_{RB,L2}$ by summarizing all components.

$$W_{RB,L2} = G_{prot,BR\_CI}\cdot M_{prot} + G_{lip,BR\_CI}\cdot M_{lip} + G_{ch,BR\_CI}\cdot M_{ch} + G_{inert,BR\_CI}\cdot M_{inert} + G_{BIO,BR\_CI}\cdot M_{BIO} \qquad \text{(I.20)}$$

To determine the CHONSP composition of the RB the composition of the components is used (equations I.21 and I.22).

$$E_{RB\_1} = E_{prot}\cdot G_{prot,BR\_CI} + E_{lip}\cdot G_{lip,BR\_CI} + E_{ch}\cdot G_{ch,BR\_CI} + E_{inert}\cdot G_{inert,BR\_CI} + E_{BIO}\cdot G_{BIO,BR\_CI} \qquad \text{(I.21)}$$

$$E_{RB} = \frac{E_{RB\_1}}{C_{RB\_1}} \qquad \text{(I.22)}$$

→ Both equations I.23 and I.24 account for each element E

After obtaining the CHONSP composition of the new RB the molecular weights can be determined, followed by the mass flow through the use of the molar flow (mol/s) and leading to the determination of the concentration of the outflows.

These values are used to calculate the quantity of water associated to this biomass, $f_{H2O,RB,Lout}$.

The mass flow, in dry weight, of the residual biomass that enters the bioreactor is:

$$W_{RB,Lin} = c_{RB,\ Lin}\cdot Q_{Lin}\cdot M_{RB} \qquad \text{(I.23)}$$

The quantity of non-degradable biomass is:

$$W_{RB\_ND} = G_{prot,BR\_CI}\cdot M_{prot} + G_{lip,BR\_CI}\cdot M_{lip} + G_{ch,BR\_CI}\cdot M_{ch} + G_{inert,BR\_CI}\cdot M_{inert} \qquad \text{(I.24)}$$

The water contained in the residual biomass at the input is:

$$W_{H2O,RB,Lin} = \frac{W_{RB}}{1 - f_{H2O,RB,Lin}}\cdot f_{H2O,RB,Lin} \qquad \text{(I.25)}$$

→ $f_{H2O,RB,Lin}$ is the fraction of water in the damp residual biomass that enters the bioreactor

The quantity of water contained in the damp residual biomass at the output has considered the water from the micro-organism's biomass that has been produced and was not degraded:

$$W_{H2O,RB,Lout} = \frac{W_{H2O,RB,Lin}}{W_{RB,Lin}} \cdot W_{RB\_ND} + \frac{G_{BIO} \cdot M_{BIO}}{1 - f_{H2O,BIO}} \cdot f_{H2O,BIO} \quad \text{(I.26)}$$

Therefore, the mass fraction of water in the damp biomass leaving the bioreactor is:

$$f_{H2O,RB,Lout} = \frac{W_{H2O,RB,Lout}}{W_{H2O,RB,Lout} + W_{RB,Lout}} \quad \text{(I.27)}$$

3.6.3 Compartment II: Photo-Heterotrophic Reactor (BR_CII)

3.6.3.1 Description

The volatile fatty acids that are a product of Compartment I are degraded in this reactor by the use of the micro-organism *Rhodobacter rubrum*:

$$VFA + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow \ BIOMASS\_2 + CO_2 + H_2O$$

Light is used as an energy source, which leads to a production of biomass, carbon dioxide and water.

As shown in Figure 3-6 the modelled reactor has a gas and liquid inlet as well as a gas and liquid outlet.

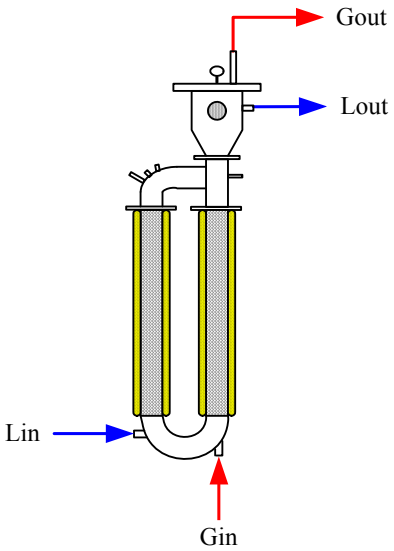


Figure 3-6: Reactor of Compartment II

The objective of the model is to obtain the concentration and volume flow rates in the output of the reactor. The procedure is very similar to that of BR_CI:

1) Calculate the composition of the biomass *R. rubrum*, and the molecular weights of biological macromolecules.
2) Calculate the stoichiometry and generation terms for each sub-process
3) Calculate the overall generation term
4) Calculate the volume flow rates and concentrations of the reactor output (balances and balances field)

3.6.3.2 Assumptions

- The bioreactor works at 30ºC and at a pH of 6,9
- The generation term is calculated through the experimental conversions of the each VFA
- The gas and liquid phases that abandon the bioreactor are in equilibrium
- The bioreactor is always illuminated

3.6.3.3 Operational Data

Reactor Parameter	Description	Value	Units
pH	pH conditions	6,9	-
Pr	Reactor Pressure	101325	Pa
R	Gas constant	8,31	J/(K mol)
T	Temperature of the bioreactor	303	K

Table 3-19: Parameter and characteristics of BR_CII

Name	Description	Value	Units
X_{VFA}	Conversion of each VFA; the moles of VFA reacting per mole of initial VFA	0,5 - 1	-

Table 3-20: Production Data of BR_CII

Note:
The sub-index “VFA” (in Table 3-20) represents each volatile fatty acid: acetic, propionic, butyric, valeric and caproic.

Name	Description	Value Ranges	Units
$(CHONSP)_{m\_Rr}$	Composition of the macromolecule "m" of *R. rubrum*; the moles of the macromolecule "m" for each mole of the macromolecule "m"	Assumptions according to [R28]: $(CH_{1.5685}O_{0.3061}N_{0.2694}S_{0.006361})_{prot}$ $(CH_{1.9223}O_{0.2153})_{lip}$ $(CH_{1.5405}O_{0.5135})_{ch}$ $(CH_{1.2295}O_{0.7256}P_{0.1043})_{RNA}$ $(CH_{1.2585}O_{0.6205}N_{0.3961}P_{1.034})_{DNA}$	-
$f_{H2O,\,Rr}$	Mass fraction of the water in the damp biomass of R. rubrum	0.5-0.97	-
f_{m_Rr}	Mass fraction of the biological macromolecule "m_Rr" in the dry biomass of R. rubrum	0-1	-

Table 3-21: R. rubrum biomass characteristics

Note:
The sub-index “m_Rr” (in Table 3-21) represents each main biological macromolecule of *R. rubrum*: DNA, RNA, carbohydrates, lipids and proteins.

3.6.3.4 Reactions, Stoichiometry and Generation Term

The stoichiometric coefficients are recalculated for each simulation, instead of defining a fixed stoichiometric equation. That choice has been made to take into account a variable composition of the biomass, which is dependent on the light irradiation, for each simulation.

Thus, the operation data needed for this calculation are the mass flow rate of protein, lipids, carbohydrates, DNA and RNA contained in the biomass of *R. rubrum* and the composition of each of these macromolecules. Through equations II.1 and II.2, the CHONSP composition of the *R. rubrum* biomass is determined.

$$E_{Rr\_1} = \sum_{m\_Rr} E_{m\_Rr} \cdot \frac{f_{m\_Rr}}{M_{m\_Rr}} \quad \text{(II.1)}$$

→ with $m\_Rr \in \{DNA, RNA, ch, lip, prot\}$

$$E_{Rr} = \frac{E_{Rr\_1}}{C_{Rr\_1}} \quad \text{(II.2)}$$

→ The equations II.1 and II.2 account for each element E. These are the values a, b, c, d, e and f, respectively.

There is a chemical reaction for each of the volatile fatty acids, which are independent from each other [R28]. For the stoichiometric resolution there are no further information required since there are six elements (C, H, O, N, S, P) and six undetermined stoichiometric coefficients.

The reactions that take place are listed below (stoichiometric coefficients are unknown):

Degradation of Acetic Acid

$$C_2H_4O_2 + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow \lfloor C_aH_bO_cN_dS_fP_g \rfloor_{Rr} + CO_2 + H_2O$$

Degradation of Propionic Acid

$$C_3H_6O_2 + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow \lfloor C_aH_bO_cN_dS_fP_g \rfloor_{Rr} + CO_2 + H_2O$$

Degradation of Butyric Acid

$$C_4H_8O_2 + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow \lfloor C_aH_bO_cN_dS_fP_g \rfloor_{Rr} + CO_2 + H_2O$$

Degradation of Valeric Acid

$$C_5H_{10}O_2 + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow \lfloor C_aH_bO_cN_dS_fP_g \rfloor_{Rr} + CO_2 + H_2O$$

Degradation of Caproic Acid

$$C_6H_{12}O_2 + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow \lfloor C_aH_bO_cN_dS_fP_g \rfloor_{Rr} + CO_2 + H_2O$$

By the use of the stoichiometry the generation term can be calculated through the equations 11 and 12 in section 3.6.1.1 (the conversion will be referred to each VFA).

3.6.4 Compartment III: Nitrifying Reactor

3.6.4.1 Description

Compartment III has the function to transform ammonia into nitrate which will be used as nutrient for the autotrophy organisms. It is an aerobic process carried out by *Nitrosomonas europaea* and *Nitrobacter winogradskyi* micro-organisms.

$$O_2 + CO_2 + NH_3 + H2SO4 + H_3PO_4 \rightarrow BIOMASS\_3 + HNO_3 + H_2O$$

N. eurepaea and *N. winogradkyi* excess biomass must be removed from the reactor to avoid their decay and the production of unwanted substrates as well as to be able to work in steady state.

The bioreactor has one gas and liquid inlet as well as one gas and liquid outlet, as shown in Figure 3-7.

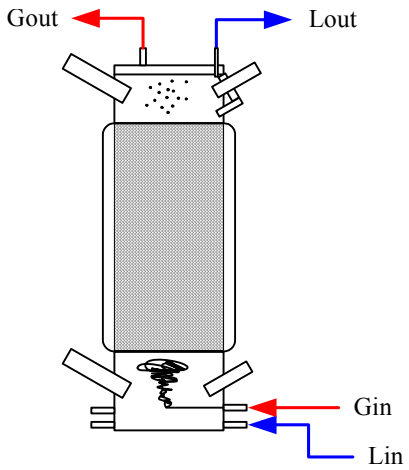


Figure 3-7: Reaction of Compartment III

The objective of the mathematical model is to gain the concentration and volume flow rates of these outputs. The stoichiometric steps are very similar to the previous reactors.

3.6.4.2 Assumptions

- The bioreactor works at 29ºC and at a pH of 8,1
- The generation term is calculated through the experimental conversions of ammonia
- The nitrite conversion is total
- The gas and liquid phases that abandon the bioreactor are in equilibrium

3.6.4.3 Operational data

Reactor Parameter	Description	Value	Units
pH	pH Concentration	8,1	-
Pr	Reactor Pressure	101325	Pa
R	Gas Constant	8,32	J/(K mol)
T	Reactor Temperature	302	K

Table 3-22: Parameters and characteristics of BR_CIII

Symbol	Description	Value	Units
Tm_{Ne}	Maintenance of *Nitrobacter*. This is the molar fraction of oxidized to nitrite maintaining the *Nitrobacter* bacteria.	0,76 [R35]	-
Tm_{Nw}	Maintenance of *Nitrosomonas*. The molar fraction of oxidized ammonia maintaining Nitrosomonas bacteria.	0,81 [R35]	-
X_{HNO2}	Conversion of nitrite. The moles of nitrite assimilated by *Nitrobacter* per mole of initial nitrite.	1	-
X_{NH3}	Conversion of ammonia. The moles of ammonia assimilated by *Nitrosomonas* per mole of initial ammonia.	0,5 – 0,9	-

Table 3-23: Production data of BR_CIII

Symbol	Description	Value	Units
$(CHONSP)_{New}$	Composition of *N. Eurepaea* and *N. Winogradkyi*. Fixed data, fixed stoichiometry.	$(CH_{1.6147}O_{0.3906}N_{0.1994}S_{0.0035})_{New}$ [R37]	-
$f_{H2O,\ New}$	Mass fraction of water in the damp biomass	0,5 - 1	-
f_{m_New}	Mass fraction of biological macromolecules "m_New" in the dry biomass	0 - 1	-

Table 3-24: Data on biomass. N. Eurepaea and N. Winogradkyi

Note:
The sub-index “m_New” (in Table 3-24) represents the major biological macromolecules of the *Nitrosomonas* and *Nitrobacter* biomass: DNA, RNA, carbohydrates, lipids and proteins.

3.6.4.4 Reactions, Stoichiometry and Generation term

The *Nitrosomonas* and *Nitrobacter* strains perform the transformation of NH_3 into NO_3. For each strain, three reactions occur: one for growth, one for maintenance and one for decay [R37] which is prevented in the bioreactor. Nitrification is a result of the oxidation of ammonia and nitrite as well as of the growth of the micro-organisms. Therefore, for each crop both reactions have been taken into account, the growth and maintenance. It shall be noted that the maintenance reaction for the oxidation of the metabolism has equal or higher influence on the production rate than the micro-organism growth.

Nitrosomonas:

- Growth:

$$CO_2 + 4.5341\,NH_3 + 0.0035\,H_2SO_4 + 0.0089\,H_3PO_4 + 5.42685\,O_2 \rightarrow [CH_{1.6147}O_{0.3906}N_{0.1994}S_{0.0035}P_{0.0089}]_{New} + 4.3347\,HNO_2 + 3.8433\,H_2O$$

- Maintenance:

$$NH_3 + 1.5\,O_2 \rightarrow HNO_2 + H_2O$$

Nitrobacter:

- Growth:

$$CO_2 + 0.1994\ NH_3 + 0.0035\ H_2SO_4 + 0.0089\ H_3PO_4 + 6.5105\ O_2 + 15.1714\ HNO_2 + 0.4914\ H_2O \rightarrow [CH_{1.6147}O_{0.3906}N_{0.1994}S_{0.0035}P_{0.0089}]_{New} + 15.1714\ HNO_3$$

- Maintenance:

$$HNO_2 + 0.5\,O_2 \rightarrow HNO_3$$

The molar inflow of ammonia $Z_{NH3,in}$ can be determined, through the concentration of ammonia and the volumetric flow at the inlet of the bioreactor. Through the ammonia conversion the moles of oxidized ammonia $G_{NH3,Ne}$ can be obtained. The molar flow of ammonia consumed by the growth, and those consumed by the maintenance, can be determined, using the maintenance rate (see equations III.1 III.2 and III.3).

$$G_{NH3,\,Ne} = -Z_{NH3,\,Ein} \cdot X_{NH3} \qquad \text{(III. 1)}$$

$$G^{man}_{NH3,\,Ne} = G_{NH3,\,Ne} \cdot Tm_{Ne} \qquad \text{(III. 2)}$$

$$G^{gr}_{NH3,\,Ne} = G_{NH3,\,Ne} \cdot (1 - Tm_{Ne}) \qquad \text{(III. 3)}$$

The generation of the remaining compounds for both the *Nitrosomonas* growth and maintenance can be determined through stoichiometry. It is important to take into account that oxygen, nitrite and water participate in both reactions.

For the generation of each compound for growth and maintenance of *Nitrobacter winogradkyi* the equations are similar, only with nitrite as reactant under known conversion (given as operational conditions).

The overall generation term of each compound in the bioreactor is the sum of all generation terms of each sub-process:

$$G_{i,\ BR\_CIII} = \sum G^{man}_{i,\ Ne} + \sum G^{gr}_{i,\ Ne} + \sum G^{man}_{i,\ Nw} + \sum G^{gr}_{i,\ Nw} \qquad \text{(III. 4)}$$

→ for each compound "i". For the compounds "i" that do not participate in the nitrification their stoichiometric coefficient is zero and, consequently, their generation term is zero.

3.6.5 Compartment IVa: Photosynthetic Reactor

3.6.5.1 Description

This bioreactor (see Figure 3-8) has the objective to generate edible biomass by means of a photosynthetic process. Thus, compartment IVa is able to produce edible biomass in the form of the algae species *Arthrospira platensis* and oxygen by using the basic nutrients (phosphates, sulphates and nitrates), carbon dioxide as a carbon source and light as energy source.

$$HNO_3 + H_2SO_4 + H_3PO_4 + CO_2 \rightarrow BIOMASS\_4a + O_2 + H_2O$$

The mathematical model has a gas and liquid inlet and a gas and liquid output. It is designed to determine the concentrations and volume flow rates of the outputs from the bioreactor.

Therefore, the following steps are defined:

1. Calculate the composition of the *Arthrospira platensis*, and the molecular weights of biological macromolecules: proteins, carbohydrates and lipids
2. Calculate the stoichiometry and generation term for each component
3. Calculate the volume flow rates and concentrations of the output of the reactor (balances and balances field)

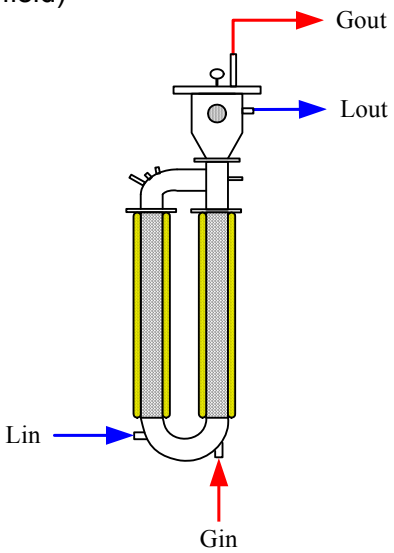


Figure 3-8: Reactor of Compartment CIVa

3.6.5.2 Assumptions

- The bioreactor works at 36ºC and at a pH of 9,5
- The generation term is calculated through the experimental conversions of the nitrate
- The gas and liquid phases that abandon the bioreactor are in equilibrium
- The bioreactor is always illuminated, which intensity is compressed between 60 and 120 W / m^2

3.6.5.3 Operational Data

Reactor Parameter	Description	Value	Units
pH	pH Concentration	9,5	-
Pr	Reactor Pressure	101325	Pa
R	Gas Constant	8,32	J/(K mol)
T	Reactor Temperature	309	K

Table 3-25: Parameters and Characteristics of BR_CIVa

Symbol	Description	Value	Units
F_o	Light intensity	60 - 120	W / m^2
X_{HNO3}	Conversion of nitrate. The moles of nitrate reacting per mole of initial nitrate	0,5 - 1	-

Table 3-26: Production Data of BR_CIVa

Symbol	Description	Value	Units
$(CHONSP)_{m\_Ap}$	Composition of biological macromolecules "m_Ap" comprising of *Arthrospira*. The moles of each element of the macromolecule "m" for each mole of macromolecule "m".	?	-
$f_{H2O,\ Ap}$	Mass fraction in water in the damp *Arthrospira* biomass	0,5 - 1	-

Table 3-27: Data on the biomass of A. platensis

Note:

The sub-index “m_Ap” (in Table 3-27) represents the major biological macromolecules of the *Arthrospira*: proteins, lipids, carbohydrates, DNA and exopolysacarids.

3.6.5.4 Reactions, Stoichiometry and Generation Term

The biomass production in this bioreactor is parameter dependent on the intensity of light. Thus, the first step is to know the composition of *A. platensis* to further calculate the stoichiometric coefficients.

The relationship between the percentage of biomolecules of seaweed and the intensity of the light, F_0 is described in Table 3-28.

Biomolecules	Mass Fraction, f_{m_Ap}
Carbohydrates	$f_{ch} = 0.96 \cdot (1 - \%_{prot} - \%_{lip} - \%_{ex})$
DNA	$f_{DNA} = 4 \cdot (1 - \%_{ex})$
Exopolysaccharid	$f_{ex} = 0.110 \cdot F_o + 9.028$
Lipids	$f_{lip} = 9.6$
Proteins	$f_{prot} = 0.96 \cdot (-0.01067 \cdot F_o + 66.088)$

Table 3-28: Arthrospira composition in function of the light intensity, according to [R36]

With the value F_0 and through the equations in Table 3-28 the fraction of each of the biological macromolecules of *Arthrospira* can be calculated. If the composition of CHONSP of each macromolecule (proteins, lipids, carbohydrates, DNA and Exopolysaccharides) is known, then the composition CHONSP of *Arthrospira* can be calculated (equations IVa.1 and IVa.2).

$$E_{Ap\_1} = \sum_{m\_Ap} E_{m\_Ap} \cdot \frac{f_{m\_Ap}}{M_{m\_Ap}} \qquad \text{(IVa.1)}$$

→ with $m\_Ap \in \{DNA, RNA, ch, ex, lip, prot\}$

$$E_{Ap} = \frac{E_{Ap\_1}}{C_{Ap\_1}} \qquad \text{(IVa.2)}$$

→ The equations IVa.2 and IVa.2 account for each element E. These are the values a, b, c, d, e and f, respectively, which are used for calculating the generation and are represented in Table 3-29

The stoichiometric coefficients of the reaction can be calculated as in the previous cases, since it takes six coefficients and six elements E (see the reaction and Table 3-29).

The reaction that takes place is (stoichiometric coefficients are unknown):

$$CO_2 + HNO_3 + H_2SO_4 + H_3PO_4 \rightarrow \left[C_aH_bO_cN_dS_fP_g\right]_{Arthrospira} + O_2 + H_2O$$

It has to be noted that except for Y_{CO2} = -1 the stoichiometry coefficients are unknown.

Compounds, i	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
CO_2	-1	1	0	2	0	0	0
HNO_3	$Y_{HNO3, S}$	0	3	0	0	0	0
H_2O	$Y_{H2O, S}$	0	2	0	0	0	0
H_2SO_4	$Y_{H2SO4, S}$	0	2	4	0	1	0
H_3PO_4	$Y_{H3PO4, S}$	0	3	4	0	0	1
O_2	$Y_{O2, S}$	0	0	2	0	0	0
Arthrospira Biomass	$Y_{BIO4a, S}$	a	b	c	d	f	g

Table 3-29: Stoichiometry and composition of the Arthrospira's photosynthesis process

The generation term is calculated by equation 11 and 12 and referring to the conversion of nitrate assimilation, X_{HNO3}.

3.7 MELiSSA Chambers Mathematical Model Description

There are two chambers in MELiSSA, one for the Crew and another for the Higher Plants. In fact, these chambers can be treated as if they were reactors, but with a specific separation between the gas and liquid phases. Therefore, the mass balances, equations 3, 4 and 5 in section 3.6, are valid.

3.7.1 Compartment IVb: Higher Plant Chamber (HPC)

3.7.1.1 Description

The function of the HPC is the provision of life support elements including food production in particular, but also CO_2 fixation, O_2 generation and potable water production.

The process that takes place is very similar to the process in compartment IVa, since both are a photosynthetic process. Thus, plants use the basic nutrients as nitrogen, sulphur and phosphor source, CO_2 as carbon source and light as energy source in order to produce biomass:

$$HNO_3 + H_2SO_4 + H_3PO_4 + HNO_3 + NH_3 + CO_2 + H_2O \rightarrow BIOMASS\_4b + O_2$$

The plants composition (macromolecule mass fraction and composition) has been built up by a pool of 8 plants: tomato, potatoes, salad, wheat, rice, soybean, onion and spinach.

The chamber is made of two inputs, gas and liquid (hydroponics environment), and three outputs, gas, liquid and solid. The solid output corresponds to the higher plants, while the liquid output is the liquid surplus of the chamber. The gas output is for the produced oxygen (see Figure 3-9).

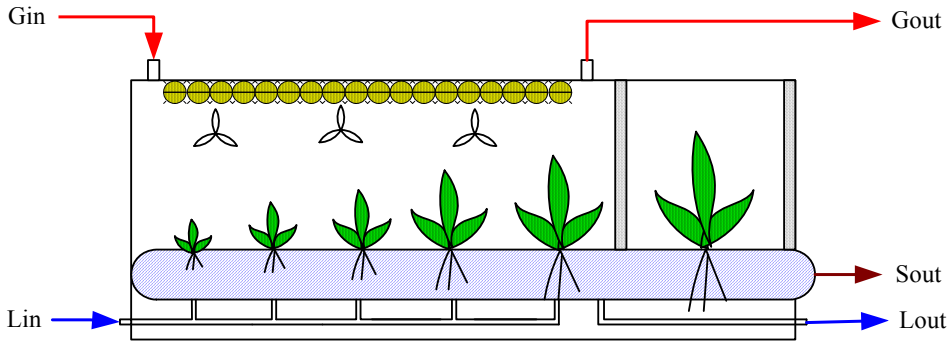


Figure 3-9: High Plants Chamber

The model's objective is to calculate the concentration and the volumetric flows at the outlet, the CHONSP composition of the global biomass produced (differentiated between edible and non edible), the required area for the production of each crop, as well as the total required area. To simplify, it is considered that the BR_CIVa is assumed to be constantly illuminated so that the plants are constantly performing photosynthesis.

The steps for the calculation are:

1. Calculate each plant composition and their molecular weight.
2. Calculate each plant's production, as well as the total biomass production, both edible and non edible (residual).
3. Calculate the total edible composition and the total residual composition.
4. Calculate the required area for the production of each plant and, therefore, the total area necessary.
5. Calculate the stoichiometry and the generation terms for each component in each sub-process and for each plant type.
6. Calculate the total generation term for each component.
7. Calculate the volumetric flows and the concentration at the chamber outline.

3.7.1.2 Assumptions

- The chamber works between 20 and 26ºC and at neutral pH
- The chamber is always illuminated
- The CHONSP composition of each bio-molecule of each plant, as well as the mass fraction of each bio-molecule in each plant are given by [R35]
- The area required for the production of each edible dry plant and the water transpired for each specie are given by [R35]
- The biomass plants density is equal to the water density

3.7.1.3 Operational Data

Reactor parameters	Description	Value	Units
Pr	Pressure	101325	Pa
R	Ideal Gas Constant	8,32	J/(K mol)
T	Bioreactor Temperature	293 - 299	K

Table 3-30: Parameters and characteristics of the HPC

Symbol	Description	Value	Units
$(f_{com,com})_v$	Mass fraction of the edible part of a plant "v" in total edible biomass (dry weight)	See [R35]	-
$(f_{HNO3,NH3})_v$	kg of HNO3 per kg of NH3 for each plant "v"	See [R35]	-
W_{com}	Quantity of total edible biomass to be produced (in dry weight)	TBD	kg/s

Table 3-31: HPC production data

Data on plants "v"	Description	Units
$(CHONSP)_{m\_HPc,v}$	Composition of macromolecules "m_HPc" of the higher plants "v" in element of moles of the macromolecule "m_HPc" for each mole of macromolecule "m"	-
$(CHONSP)_{re,v}$	Composition of the residue from the plant "v" in moles of the element (CHONSP) of the residue per mole of residue	-
CY_v	crop yield of harvested plant "v" (in dry weight)	$(kg)_{v\ dried}/(m^2 s)$
$(f_{H2O,com})_v$	Mass fraction of water in damp edible part of higher plant's "v" biomass	-
$(f_{H2O,re})_v$	Mass fraction of water in damp residual biomass of higher plants "v"	-
$(f_{m\_HPc,com})_v$	Mass fraction of macromolecules "m_HPc" on the dry mass of comestible higher plants "v"	-
$(f_{re,com})_v$	Mass fraction of the residual portion of the plant in the edible portion of the plant "v" in kilograms of waste per kg of edible plant "v" (dry weight)	-
TW_v	Transpired water per plant "v"	$(kg)_{water}/(m^2 s)$

Table 3-32: Data about vegetables

Notes:

- The sub-index "v" (in Table 3-31 and in Table 3-32) represents each kind of vegetable: tomato, potatoes, salad, wheat, rice, soybean, onion and spinach.
- The sub-index "m_HPc" (in Table 3-32) represents each main biological macromolecules of the comestible part of the plants: DNA, RNA, carbohydrates, fibres, proteins, lipids and saturate lipids.

The production data and the vegetables composition data are values determined with the aim to achieve the nutritive requirements for the crew.

3.7.1.4 CHONSP Composition of Each Plant

To solve the stoichiometry it is necessary to calculate first the CHONSP composition of each plant that participates in the process, based on the data given in Table 3-32. With the eatable CHONSP composition of each plant (equations IVb.1 and IVb.2) the total CHONSP (comestible + residual) for each one can be calculated (equations IVb.3 and IVb.4).

$$E_{com\_1,v} = \sum_{m\_HPc} E_{m\_HPc,v} \cdot \frac{(f_{m\_HPc,com})_v}{M_{m\_HPc}} \qquad \text{(IVb.1)}$$

$$\rightarrow\ m\_HPc \in \{DNA, RNA, ch, fib, lip, lipsat, prot\}$$

$$E_{com,v} = \frac{E_{com\_1,v}}{C_{com\_1,v}} \qquad \text{(IVb.2)}$$

$$E_{v\_1} = \frac{E_{com,\,v}}{M_{com,\,v}} + \frac{E_{re,\,v}}{M_{re,\,v}} \cdot (f_{re,\,com})_v \qquad \text{(IVb.3)}$$

$$E_v = \frac{E_{v\_1}}{C_{v\_1}} \qquad \text{(IVb.4)}$$

→ for each element E and each plant “v”, with
$v \in \{\text{tomato}, \text{potatoes}, \text{salad}, \text{wheat}, \text{rice}, \text{soybean}, \text{onion}, \text{spinach}\}$.

Num.) plant	Function / File	Composition used to defined crops
1) Tomato	Composition_tomato.m Composition_tomato.mat	**Proteins : 14.75 %** in dry edible [$CH_{1.46731}O_{0.46578}N_{0.23469}S_{0.000205}$] **Lipids : 14.75 %** in dry edible (composed of 22.84% of Lipids 1) Lipids 1 : [$CH_2O_{0.1231}$] Lipids 2 : [$CH_{1.81116}O_{0.1383}$] **Carbohydrates : 14.75 %** in dry edible [$CH_{1.8958}O_{0.9924}$] **Fibres : 14.75 %** in dry edible [$CH_{1.6560}O_{0.8280}$] **Waste : 955%** of dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 93.6 %** of fresh mass **Water content of waste part : 50 %** of fresh mass Crop Yield : 18 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
2) Potatoes	Composition_potato.m Composition_potato.mat	**Proteins : 10.17 %** in dry edible [$CH_{1.50971}O_{0.38347}N_{0.25300}S_{0.000425}$] **Lipids : 0.55 %** in dry edible (composed of 22.84% of Lipids 1) Lipids 1 : [$CH_2O_{0.1214}$] Lipids 2 : [$CH_{1.74071}O_{0.11164}$] **Carbohydrates : 76.77 %** in dry edible [$CH_{1.6686}O_{0.8436}$] **Fibres : 12.51 %** in dry edible [$CH_{1.6513}O_{0.8257}$] **Waste : 49.96%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 79.5 %** of fresh mass **Water content of waste part : 50 %** of fresh mass Crop Yield : 33 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
3) Wheat	Composition_wheat.m Composition_wheat.mat	**Proteins : 13.8 %** in dry edible [$CH_{1.5}O_{0.359}N_{0.242}S_{0.007}$] **Lipids : 2.35 %** in dry edible (composed of 19.68% of Lipids 1) Lipids 1 : [$CH_2O_{0.1189124}$] Lipids 2 : [$CH_{1.8786}O_{0.11774}$] **Carbohydrates : 71.73 %** in dry edible [$CH_{1.6761}O_{08381}$] **Fibres : 12.12 %** in dry edible [$CH_{1.6667}O_{0.8333}$] **Waste : 152.50%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 13.44 %** of fresh mass **Water content of waste part : 12 %** of fresh mass Crop Yield : 33 d dry edible / m^2.day Transpiration Water : 2.9 kg / m^2 .day
4) Rice	Composition_rice.m Composition_rice.mat	**Proteins : 8.42 %** in dry edible [$CH_{1.53355}O_{0.35016}N_{0.25885}S_{0.00626}$] **Lipids : 2.57 %** in dry edible (composed of 29.9% of Lipids 1) Lipids 1 : [$CH_2O_{0.1231}$] Lipids 2 : [$CH_{1.81116}O_{0.1231}$] **Carbohydrates : 85.66 %** in dry edible [$CH_{1.8957}O_{0.99239}$] **Fibres : 3.35 %** in dry edible [$CH_{1.6667}O_{0.8333}$] **Waste : 119.77%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 13.26 %** of fresh mass **Water content of waste part : 15 %** of fresh mass Crop Yield : 4 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day

Figure 3-10: Part 1 Composition of higher plants used in HPC according to [R35]

Num.) plant	Function / File	Composition used to defined crops
5) Salad	Composition_salad.m	**Proteins : 30.56 %** in dry edible [$CH_{1.64190}O_{0.19376}N_{0.24639}S_{0.00352}$]
	Composition_salad.mat	**Lipids : 5.38 %** in dry edible (composed of 22.68% of Lipids 1) Lipids 1 : [$CH_2O_{0.12355}$] Lipids 2 : [$CH_{1.725848}O_{0.111758}$] **Carbohydrates : 26.89 %** in dry edible [$CH_{1.7962}O_{0.9919}$] **Fibres : 37.1 %** in dry edible [$CH_{1.6537}O_{0.8268}$] **Waste : 85.61%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 95.27 %** of fresh mass **Water content of waste part : 80%** of fresh mass Crop Yield : 6 d dry edible / m^2.day Transpiration Water : 1.2 kg / m^2 .day
6) Soybean	Composition_soybean.m Composition_soybean.mat	**Proteins : 46.14 %** in dry edible [$CH_{1.53073}O_{0.34292}N_{0.25367}S_{0.00667}$] **Lipids : 24.76 %** in dry edible (composed of 13.9% of Lipids 1) Lipids 1 : [$CH_2O_{0.1212}$] Lipids 2 : [$CH_{1.83076}O_{0.11495}$] **Carbohydrates : 8.34 %** in dry edible [$CH_{1.8822}O_{0.9411}$] **Fibres : 20.76 %** in dry edible [$CH_{1.60}O_{0.80}$] **Waste : 55.81%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 10.42 %** of fresh mass **Water content of waste part : 50%** of fresh mass Crop Yield : 15 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
7) Onion	Composition_onions.m Composition_onions.mat	**Proteins : 12.09 %** in dry edible [$CH_{1.64586}O_{0.17818}N_{0.34576}S_{0.00448}$] **Lipids : 2.42 %** in dry edible (composed of 47% of Lipids 1) Lipids 1 : [$CH_2O_{0.1210}$] Lipids 2 : [$CH_{1.76406}O_{0.1111}$] **Carbohydrates : 56 %** in dry edible [$CH_{1.8551}O_{0.9716}$] **Fibres : 29.5 %** in dry edible [$CH_{1.6560}O_{0.8280}$] **Waste : 157.87%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 89.44 %** of fresh mass **Water content of waste part : 50%** of fresh mass Crop Yield : 22.5 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day
8) Spinach	Composition_spinach.m Composition_spinach.mat	**Proteins : 47.82 %** in dry edible [$CH_{1.62780}O_{0.19299}N_{0.24837}S_{0.01169}$] **Lipids : 5.69 %** in dry edible (composed of 14.61% of Lipids 1) Lipids 1 : [$CH_2O_{0.1244}$] Lipids 2 : [$CH_{1.70827}O_{0.11226}$] **Carbohydrates : 11.57 %** in dry edible [$CH_{1.6154}O_{0.9684}$] **Fibres : 34.91 %** in dry edible [$CH_{1.6467}O_{0.8233}$] **Waste : 157.55%** in dry edible [$CH_{1.43}O_{0.62}N_{0.017}S_{0.007}$] **Water content of Edible part : 9756 %** of fresh mass **Water content of waste part : 80%** of fresh mass Crop Yield : 21 d dry edible / m^2.day Transpiration Water : 5 kg / m^2 .day

Figure 3-11: Part 2 Composition of higher plants used in HPC according to [R 35]

3.7.1.5 Plants Production

In the equations below the total production (comestible + residue) of each plant, W_v (equation IVb.6), the comestible quantity of each one, $W_{com,v}$ (equation IVb.5), as well as the wastes generated, $W_{re,v}$ (equation IVb.7) are calculated. All values are given in dry weight, without taking into account the water they contain.

$$W_{com,\,v} = W_{com} \cdot (f_{com,\,com})_v \qquad \text{(IVb.5)}$$

$$W_v = \frac{W_{com,v}}{1 - \frac{(f_{re,com})_v}{1 + (f_{re,com})_v}} \quad \text{(IVb.6)}$$

$$W_{re,v} = W_v \cdot \frac{(f_{re,com})_v}{1 + (f_{re,com})_v} \quad \text{(IVb.7)}$$

→ These equations account for each plant "v".

The total production of residues is:

$$W_{re} = \sum_v W_{re,v} \quad \text{(IVb.8)}$$

3.7.1.6 Total Edible and Total Residual Part CHONSP Composition

In section 3.7.1.4 the CHONSP composition of the comestible and residual part for each vegetable has obtained. Once the production of each one is expressed, the total CHONSP composition for both, comestible and residual parts, can be calculated.

Comestible Part (HPc):

$$E_{HPc\_1} = \sum_v E_{com,v} \cdot \frac{W_{com,v}}{M_{com,v}} \quad \text{(IVb.9)}$$

$$E_{HPc} = \frac{E_{HPc\_1}}{C_{HPc\_1}} \quad \text{(IVb.10)}$$

For the Food Treatment Unit (FTU) it is necessary to know the CHONSP composition (equation IVb.11) and the mass fraction (equation IVb.12) of the biological macromolecule "m" (carbohydrates, lipids and proteins) that form part of the global comestible biomass.

$$E_{m,HPc\_1} = \sum_v E_{m,v} \cdot (f_{m,com})_v \cdot \frac{W_{com,v}}{M_m} \quad \text{(IVb.11)}$$

$$E_{m,HPc} = \frac{E_{m,HPc\_1}}{C_{m,HPc\_1}} \quad \text{(IVb.12)}$$

→ The equations IVb.9, IVb.10, IVb.11 y IVb.12 account for each element E.

$$f_{m,HPc} = \frac{\sum_v (f_{m\_HPc,com})_v \cdot W_{com,v}}{W_{com}} \quad \text{(IVb.13)}$$

→ The equation accounts for each macromolecule "m" of the edible higher plants

Residual Part (HPre):

$$E_{HPre\_1} = \sum_v E_{re,v} \cdot \frac{W_{re,v}}{M_{re,v}} \quad \text{(IVb.14)}$$

$$E_{HPre} = \frac{E_{HPre\_1}}{C_{HPre\_1}} \quad \text{(IVb.15)}$$

→ The equations IVb.14 and IVb.15 account for each element E

3.7.1.7 Required Production Area

Each plant is given a yield that expresses the quantity of produced edible biomass per time unit and area, CY_v. Therefore, once the production flow of edible plant mass is known, the production area for each plant can be expressed (equation IVb.16).

$$A_v = \frac{W_{com,\,v}}{CY_v} \qquad \text{(IVb.16)}$$

→ for each plant "v"

And the total area necessary is:

$$A = \sum_v A_v \qquad \text{(IVb.17)}$$

3.7.1.8 Stoichiometry and Generation Term

As it has been explained, the plants composition (data in Table 3-32) is used to calculate the global composition of each plant, afterwards the global composition (a, b, c, d, e and f) is used in the reactions that take place.

Within the HPC each vegetal has a similar process: the carbon dioxide, nitrate, ammonia, sulphate and phosphate consumption in order to produce comestible biomass, oxygen and water:

$$CO_2 + HNO_3 + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow [C_aH_bO_cN_dS_eP_f]_{plant\ v} + O_2 + H_2O$$

As up to eight plants have been considered, there can be a maximum of eight sub-processes. The stoichiometry equation for each plant can be solved using the relation between the two nitrogen sources: HNO_3 and NH_3 (see equation IVb.18).

Thus, the stoichiometric coefficients for the production of each plant are solved the same way than in previous cases (see Table 3-33 and equations IVb.18 and IVb.19).

Compound "i"	Stoichiometric coefficient, Y	Composition					
		C	H	O	N	S	P
Biomass	$(Y_{BIO4b,\,HPC})_v$	a	b	c	d	e	f
CO_2	-1	1	0	2	0	0	0
HNO_3	$(Y_{HNO3,\,HPC})_v$	0	3	0	0	0	0
H_2O	$(Y_{H2O,\,HPC})_v$	0	2	0	0	0	0
H_2SO_4	$(Y_{H2SO4,\,HPC})_v$	0	2	4	0	1	0
H_3PO_4	$(Y_{H3PO4,\,HPC})_v$	0	3	4	0	1	1
NH_3	$(Y_{NH3,\,HPC})_v$	0	3	0	1	0	0
O_2	$(Y_{O2,\,HPC})_v$	0	0	2	0	0	0

Table 3-33: Stoichiometry and composition of the higher plants photosynthesis

$$(Y_{HNO3,\,HPC})_v = y(HNO3)_v \cdot \frac{M_{NH3}}{M_{HNO3}} \cdot (Y_{NH3,\,HPC})_v \qquad \textit{(IVb.18)}$$

→ for each plant "v"

$$\sum_i (Y_{i,\,HPC})_v \cdot E_i = 0 \qquad \text{(IVb.19)}$$

→ for each element E. The term $(Y_{i,HPC})_v$ is the stoichiometric coefficient of the compound "i" in the HPC to produce the plant "v". The compounds that participate in

the production of the plant "v" are those represented in Table 3-33. The stoichiometric coefficient for the rest of compounds is zero.

The generation of each compound can be calculated through the stoichiometry and the molecular weight of each plant:

$$(G_{i,HPC})_v = \frac{W_v}{M_v} \cdot \frac{(Y_{i,HPC})_v}{(Y_{v,HPC})_v} \qquad \textit{(IVb.20)}$$

→ for each compound "i" to produce the plant "v" in the HPC.

The global generation of each compound, except of the water:

$$G_{i,HPC} = \sum_v (G_{i,HPC})_v \qquad \text{(IVb.21)}$$

→ for each compound "i", except for H2O, in the HPC to produce the global high plants biomass.

This generation of each compound is a consequence of the production of dry biomass. Water participates in this process, and is additionally used as a liquid within the plants organs. Thus, these organisms capture a certain quantity of water.

The quantity of water (per time unit) that the residual part contains is calculated through equation IVb.22 and the water content in the comestible part through IVb.23. The total quantity of water contained in the higher plants biomass (HP) is the sum of both parts (equation IVb.24).

$$W_{H2O,HPre} = \sum_v \frac{W_{re,v}}{1-(f_{H2O,re})_v} \cdot (f_{H2O,re})_v \qquad \text{(IVb.22)}$$

$$W_{H2O,HPc} = \sum_v \frac{W_{com,v}}{1-(f_{H2O,com})_v} \cdot (f_{H2O,com})_v \qquad \text{(IVb.23)}$$

$$W_{H2O,HP} = W_{H2O,HPre} + W_{H2O,HPc} \qquad \text{(IVb.24)}$$

It is important to take into account, that plants perspire water vapour, $W_{H2O,pers}$. In effect, when plants take up the carbon dioxide of the gas phase, they expel molecules of water. This quantity is expressed by means of equation IVb.25.

$$W_{H2O,pers} = \sum_v A_v \cdot TW_v \qquad \text{(IVb.25)}$$

3.7.1.9 Compounds Distribution between the Outputs: Liquid and Gas

In contrast with the bioreactors, in the HPC no particle exchange between the liquid and gas phases occurs, since both of them are separated by the substrate of the plants. However, the plants are in contact with both phases taking the carbon dioxide from the gas and expelling oxygen and water through their leaves. Additionally, they absorb the minerals and the water from the hydroponics environment through the roots.

Therefore, in the gas phase changes in the CO_2, O_2 and H_2O moles occur; while in liquid both CO_2 and O_2 keep unaltered. Thus, one generation term for the liquid and the other for the gas can be defined.

Generation in the liquid:

$$G_{i,L} = G_{i,HPC}$$

→ for each compound "i" except for H2O, CO2, O2.

The water (H2O) of the liquid is consumed due to the production of biomass, perspiration and quantity fixed for each plant:

$$G_{H2O,\ L} = \sum (G_{H2O,\ HPC})_v - \frac{W_{H2O,\ trans}}{M_{H2O}} - \frac{W_{H2O,\ HP}}{M_{H2O}}$$

The carbon dioxide (CO2) and oxygen (O2) moles keep unchanged:

$$G_{CO2,\ L} = 0$$
$$G_{O2,\ L} = 0$$

Generation in the gas:

$$G_{i,\ G} = 0$$

→ for each compound "i", except for H2O, CO2, O2.

The gas phase is sutured of water due to the perspiration:

$$G_{H2O,\ G} = \frac{W_{H2O,\ trans}}{M_{H2O}}$$

The generation in the gas for CO2 and O2 is due to the chemical reactions that take place for the biomass production:

$$G_{CO2,\ G} = G_{CO2,\ HPC}$$
$$G_{O2,\ G} = G_{O2,\ HPC}$$

The fact that both phases, liquid and gas, are not in contact, enables separate mass balances, with $Z_{i,Lin}$ y $Z_{i,Gin}$ as the molar inflows in the liquid and gas phases (equations IVb.26 and IVb.27). For the calculation of $Z_{i,Lout}$ and $Z_{i,Gout}$, (the molar outflows in the liquid and gas phases) the mass balances for each compound (equations IVb.28 and IVb.29) is used.

$$Z_{i,\ Lin} = Q_{Lin} \cdot c_{i,\ Lin} \qquad \text{(IVb.26)}$$

$$Z_{i,\ Gin} = Q_{Gin} \cdot c_{i,\ Gin} \qquad \text{(IVb.27)}$$

$$Z_{i,\ Lout} = Z_{i,\ Lin} + G_{i,\ L} \qquad \text{(IVb.28)}$$

$$Z_{i,\ Gout} = Z_{i,\ Gin} + G_{i,\ G} \qquad \text{(IVb.29)}$$

→ for each compound "i"

To determine the volumetric flow of the gas stream, the ideal gas equation (equation IVb.30) is used while for the volumetric flow of the liquid stream the density is used which is considered constant throughout the process (equations IVb.31 and IVb.32).

$$Q_{Gout} = \frac{\sum Z_{i,\ Gout} \cdot R \cdot T}{Pr} \qquad \textit{(IVb.30)}$$

$$\rho_L = \sum c_{i,\ Lin} \cdot M_i \qquad \textit{(IVb.31)}$$

$$Q_{Lout} = \frac{\sum Z_{i,Lout} \cdot M_i}{\rho_L} \qquad \textit{(IVb.32)}$$

Finally, the concentration of each compound in both phases is expressed in the following way:

$$c_{i,Gout} = \frac{Z_{i,Gout}}{Q_{Gout}} \qquad \textit{(IVb.33)}$$

$$c_{i,Lout} = \frac{Z_{i,Lout}}{Q_{Lout}} \qquad \textit{(IVb.34)}$$

→ for each compound "i" in the two outputs: gas (Gout) and liquid (Lout)

3.7.1.10 Solid stream (High Plants)

Under the assumption that plants have the same density of water, the volumetric flow of the solid output is:

$$Q_{Sout} = \frac{W_{re} + W_{com} + W_{H2O,HP}}{1000} \qquad \text{(IVb.35)}$$

3.7.2 Compartment V: Crew Chamber

3.7.2.1 Description

Compartment V is the crew chamber. It receives food, oxygen and water and transforms it to faeces, urine and metabolism products (water and carbon dioxide).

$$\text{FOOD} + O_2 + \text{WATER} \rightarrow \text{FAECES} + \text{URINE} + CO_2 + H_2O$$

The chamber consists of four inlets and four outlets (see Figure 3-12). The gas inlet stream corresponds to the supply of breathable atmosphere, the two liquid inlet streams are the potable and hygiene water support and the solid inlet corresponds to the food input. The out flowing gas contains carbon dioxide, a product of the metabolism. The solid outlet stream contains the faeces and the two liquid outlet streams are urine and residual water.

The model objective is to obtain the concentration and the volumetric flows at the outlet. One of the assumptions in the model is that anabolism and catabolism are in dynamic equilibrium. Consequently, there is no accumulation, which means that the crew neither gains nor looses weight.

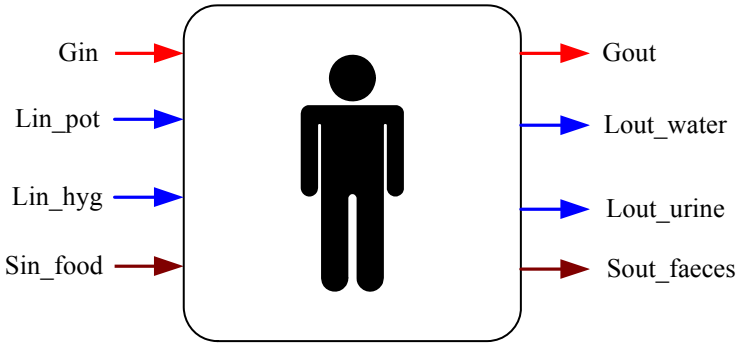


Figure 3-12: Crew Chamber

The steps for the solution are:

1. Calculate the hygiene water distribution
2. Calculate the faeces composition and its molecular weight
3. Calculate the urine composition and its molecular weight
4. Calculate the food and oxygen consumption as well as the carbon dioxide, faeces and urine production.
5. Calculate the distribution outlets: faeces, urine, gas and residual water.

3.7.2.2 Assumptions

- The chamber works between 20 and 25ºC and at atmospheric pressure
- Salts, hormones, amino acids, etc. have not been taken into account in the model
- The anabolism and the catabolism are in dynamic equilibrium
- The crew ingest all the food and all the potable water that they received
- The production of methane, hydrogen and sulphydric by the crew have not been taken into account in the model
- The faeces density and urine density is equal to the water density

3.7.2.3 Operational Data

Parameters	Description	Values	Units
Pr	Pressure	101325	Pa
R	Ideal Gas Constant	8,32	J/(K mol)
T	Chamber Temperature	296 – 298	K

Table 3-34: Parameters and characteristics of the Crew Chamber

Symbols	Description	Values	Units
$(f_{H2O})_{fc}$	Mass fraction of water contained in faeces in correspondence to the water content in the human body	0,08	-
$(f_{H2O})_{urine}$	Mass fraction of water contained in urine in correspondence to the water content in the human body	0,5	-
$(f_{H2O})_{resp}$	Mass fraction of breathed water in correspondence to the water content in the human body	0,17	-
$(f_{H2O})_{presp}$	Mass fraction of perspired water contained in urine in correspondence to the water content in the human body	0,25	-
$\%(H_2O)_d$	percentage of hygienic water that is sent to the destination "d"	?	-

Table 3-35: Distribution of water

Note:
The sub-index “d” (in Table 3-35) represents the different destination of hygienic water: faeces toilet (WC_fc), urine toilet (WC_urine) and personal hygiene (cleanliness).

Data	Description	Value	Units
$f(Abs)_m$	Mass fraction of each macromolecule “m” that is absorbed inside the human body	?	-

Table 3-36: Data about the human metabolism

Note:
The sub-index “m” (in Table 3-36) represents the main biological macromolecules of the food: carbohydrates, proteins and lipids.

Data	Description	Value	Units
$f_{cre,\ urine}$	Fraction mass creatinine in the urine (dry weight)	0,042	-

$f_{urea,\ urine}$	Mass fraction of urea in the urine (dry weight)	0,51	-
$f_{ureic,\ urine}$	Mass fraction of ureic acid in the urine (dry weight)	0,014	-

Table 3-37: Data about urine composition

3.7.2.4 Water Distribution

The crew chamber consists of two water inflows: one of hygiene and the other of potable water. The hygiene water is the one used by the astronauts for hygiene, as well as for flushing the toilets, while the potable water is free from impurities that may cause disease or harmful physiological effects and is therefore safe for human consumption and contains the required mineral salts.

The quantity of water necessary, Q_{Lin_pot} and Q_{Lin_hyg}, is a value given by the Liquid Collector and Distributor (LCD) and is a function of the crew requirements.

Within the chamber, the hygiene water has three different destinations: for the faeces flush water, for the urine flush water and for the washing water. The flows for each destination are expressed through the equation V.1:

$$Q(H_2O)_d = \%(H_2O)_d \cdot Q_{Lin\_hyg} \qquad \text{(V.1)}$$

→ for each destination "d", where $d \in \{WC\_fc, WC\_urine, cleanliness\}$

WC_fc: faeces flush water
WC_urine: urine flush water
Cleanliness: washing water

3.7.2.5 Faeces Composition

It is assumed that the astronauts ingest all the food they receive, but, only a part of this food undergoes the metabolism reactions for the energy generation.

The biological macromolecules that the human organism does not absorb are expelled in form of faeces. Therefore, if the food composition and the absorption fraction are known, it is possible to determine the faeces composition and its mass flow.

Equation V.2 expresses the quantity (in kg/s) of proteins, carbohydrates and lipids ingested by the crew:

$$W_{m,ing} = f_{m,ing} \cdot W_{ing} \qquad \text{(V.2)}$$

→ for each macromolecule "m". Both $f_{m,ing}$, and W_{ing} are values from the Food Treatment Unit (FTU).

Equation V.3 expresses the mass flow of each absorbed bio-molecule:

$$W_{m,abs} = f(Abs)_m \cdot W_{m,ing} \qquad \text{(V.3)}$$

→ The equations V.2 and V.3 account for each macromolecule "m".

The CHONSP faeces composition can be determined through the equations V.4 and V.5 since the CHONSP food composition and the CHONSP macromolecule absorbed composition are expressed in the FTU.

$$E_{fc\_1} = E_{ing} \cdot \frac{W_{ing}}{M_{ing}} - E_{prot,ing} \cdot \frac{W_{prot,abs}}{M_{prot,ing}} - E_{lip,ing} \cdot \frac{W_{lip,abs}}{M_{lip,ing}} - E_{ch,ing} \cdot \frac{W_{ch,abs}}{M_{ch,ing}} \qquad \text{(V.4)}$$

$$E_{fc} = \frac{E_{fc\_1}}{C_{fc\_1}} \quad \text{(V.5)}$$

→ for each element E of the faeces biomass. Thus, C_{fc}, H_{fc}, O_{fh}, N_{fc}, S_{fc} and P_{fc} are the values: g, h, i, j, k and m, respectively, used for the calculation of the generation.

The faeces mass flow, W_{fc}, and the macromolecule "m" mass flow is equal to the ingested flow minus the absorbed flow (equation V.6 and V.7 respectively). Consequently, the mass fraction of the faeces bio-molecules can be expressed (equation V.8).

$$W_{fc} = W_{ing} - \sum_{m} W_{m,abs} \quad \text{(V.6)}$$

$$W_{m,fc} = W_{m,ing} - W_{m,abs} \quad \text{(V.7)}$$

$$f_{m,fc} = \frac{W_{m,fc}}{W_{fc}} \quad \text{(V.8)}$$

→ The equations V.7 and V.8 account for each macromolecule "m".

3.7.2.6 Urine Composition

The urine composition varies from individual to individual, but can be done more accurately once the astronauts that participate in the mission will be known.

Urine is composed of 95% of water, and 5% compounds dissolved in the water as urea, ureic acid, creatinine, sulphates, phosphates, carbonates, inorganic salts, glucose, aminoacids, etc. Of these compounds approximately 50% is urea making it the major compound.

In the mathematic model the compounds of urine that have been considered are: urea, ureic acid, creatinine, sulphates and phosphates. In order to solve the metabolism reaction, urea, ureic acid and creatinine have been considered as one substance called Solid Urine (SU), while the sulphates and phosphates of the urine are treated as free compounds.

The CHON composition of SU is calculated from the composition of the compounds that form it (see Table 3-38) and from its mass fraction (see equations V.9 and V.10).

Compound of the Solid Urine	Composition			
	C	H	O	N
Creatinine	4	7	1	3
Urea	1	4	1	2
Ureic acid	5	4	3	4

Table 3-38: Composition of the Solid Urine compounds

$$E_{SU\_1} = E_{urea} \cdot \frac{f_{urea,urine}}{M_{urea}} + E_{ureico} \cdot \frac{f_{ureic,urine}}{M_{ureic}} + E_{cre} \cdot \frac{f_{cre,urine}}{M_{cre}} \quad \text{(V.9)}$$

$$E_{SU} = \frac{E_{SU\_1}}{C_{SU\_1}} \quad \text{(V.10)}$$

→ for each element E of the SU. Thus, C_{SU}, H_{SU}, O_{SU}, N_{SU}, are the values: n, o, p y q, that are used for the calculation of the generation.

3.7.2.7 Generation

Assuming the human body as a black box and that anabolism and catabolism are in dynamic equilibrium, the process that takes place can be summarised in the following equation of metabolism:

$$\left[C_aH_bO_cN_dS_eP_f\right]_{food} + O_2 \downarrow \left[C_gH_hO_iN_jS_kP_m\right]_{faeces} + \left[C_nH_oO_pN_q\right]_{solid\ urine} + H_2SO_4 + H_3PO_4 + CO_2 + H_2O$$

As it has been explained, the ingested food is on one hand absorbed and on the other it is expelled in faeces. The absorbed food partially supports the metabolism process obtaining basically carbon dioxide and water. The remaining part is transformed into urine (Solid Urine + H_2SO_4 + H_3PO_4).

It has to be noted that biomass is expressed in dry weight (without taking into account the water contained within the biomass cells). Therefore, water ingested (both liquid and bound in food) is excreted as urine, faeces, through perspiration and breathing. The H_2O that appears in the reaction, is the water produced by the metabolism.

The resulting gases from the chemical reactions with the stomach acids, intestinal fluids and intestinal bacteria, consist partially of carbon dioxide, methane, hydrogen and others gases like hydrogen sulphide, but due to its small proportion, it has been neglected and CO_2 is the only one considered in the model.

The food composition (a, b, c, d, e, f) is calculated in the FTU, while the faeces and the solid urine composition are expressed in the previous section. The food mass flow is also determined in the FTU, therefore its generation can be expressed considering that all food is consumed (equation V.9). The food generation can be determined through equation V10. Consequently the equation system can be solved obtaining the generation of each compound directly (see equations V.11-V.13).

Compound "i"	Generation, G	Composition					
		C	H	O	N	S	P
CO_2	$G_{CO2,\ CC}$	1	0	2	0	0	0
Faeces	$G_{hc,\ CC}$	g	h	i	j	k	m
Food	$G_{food,\ CC}$	a	b	c	d	e	f
H_2O	$G_{H2O,\ CC}$	0	2	0	0	0	0
H_2SO_4	$G_{H2SO4,\ CC}$	0	2	4	0	1	0
H_3PO_4	$G_{H3PO4,\ CC}$	0	3	4	0	1	1
O_2	$G_{O2,\ CC}$	0	0	2	0	0	0
Solid urine	$G_{orsol,\ CC}$	n	o	p	q	0	0

Table 3-39: Generation and composition for the metabolism

$$G_{food,\ CC} = -\frac{W_{ing}}{M_{food}} \quad \text{(V.11)}$$

$$G_{fc,\ CC} = \frac{W_{fc}}{M_{fc}} \quad \text{(V.12)}$$

$$\sum_i G_{i,\ CC} \cdot E_i = 0 \quad \text{(V.13)}$$

→ V.13 for each element E of each compound "i" of Table 3-39

3.7.2.8 Water Balance in Human Body

As has been explained, the ingested water is partially supplied in liquid form as drinks as well as solids form contained in food and it is excreted off the human body through urine, faeces, perspiration and breathing. Furthermore, there is a certain quantity of water produced by the metabolism, due to macromolecule breaking.

By treating the human body as a black box, the input must to be equal to the output, with the inputs being:

- Water contained in drinks, Q_{Lin_pot}
- Water contained in food $Q_{H2O,food}$
- Water product in metabolism, $Q_{H2O,met}$

} $Q_{H2O,\ body}$

And the outputs are:

- Perspired water
- Expired water
- Water in faeces
- Water in urine

} $Q_{H2O,\ body}$

This water flow can be expressed through the equation V.14:

$$Q_{H2O,body} = Q_{H2O,food} + Q_{H2O,met} + Q_{Lin\_pot} \quad \text{(V.14)}$$

With:

$$Q_{H2O,food} = \frac{W_{H2O,food}}{1000} \quad \text{(V.15)}$$

→ Where $W_{H2O,food}$, is the water flow contained in food and is provided by the FTU

$$Q_{H2O,met} = G_{H2O,CC} \cdot \frac{M_{H2O}}{1000} \quad \text{(V.16)}$$

and $Q_{H2O,pot}$ it is provided by the LCD

3.7.2.9 Outlet Stream Distribution

The Crew Chamber has four outlet streams, which are:

- Sout: Faeces (Solid output)
- Lout_urine: Urine (Liquid output)
- Gout: Gas (Gas output)
- Lout_re: Residual water (Liquid output)

3.7.2.10 Sout Stream (Faeces)

Faeces produced by the crew are sent to the correspondent toilet, where they are mixed with the necessary hygienic water. This stream is made up by faeces, water contained in faces and flush water.

Assuming the faeces density being equal to the water, the volumetric flow of this stream is expressed through equation V.17:

$$Q_{Sout} = Q_{H2O,\ body} \cdot (f_{H2O})_{fc} + \frac{W_{fc}}{1000} + Q(H_2O)_{WC\_fc} \quad \text{(V.17)}$$

with a faeces concentration given by V.18:

$$c_{fc,Sout} = \frac{G_{fc,CC}}{Q_{Sout}} \quad \text{(V.18)}$$

and a water concentration given by V.19:

$$c_{H2O,\ Sout} = \frac{(Q_{H2O,body} \cdot (f_{H2O})_{fc} + Q(H_2O)_{WC\_fc}) \cdot \frac{1000}{M_{H2O}}}{Q_{Sout}} \quad \text{(V.19)}$$

3.7.2.11 Lout_urine Stream

The assumption that urine is composed by a component called solid urine, as well as sulphuric and phosphoric acids, has been explained. Solid urine is consisting of urea, ureic acid and creatinine and its CHON composition, as expressed in section 3.7.2.6. The CHONSP global composition of urine, in dry weight, can be expressed (see and equations V.20 and V.21) through the generation term of each compound.

Compound, i	Generation, G	Composition					
		C	H	O	N	S	P
H_2SO_4	$G_{H2SO4,CC}$	0	2	4	0	1	0
H_3PO_4	$G_{H3PO4,\ CC}$	0	3	4	0	0	1
Solid Urine	$G_{SU,\ CC}$	n	o	p	q	0	0

Table 3-40: Urine composition

$$E_{urine\_1} = \sum_i G_{i,\ CC} \cdot E_i \quad \text{(V.20)}$$

→ "i" belongs to each compound shown in Table 3-40

$$E_{urine} = \frac{E_{urine\_1}}{C_{urine\_1}} \quad \text{(V.21)}$$

→ The equations V.22 and V.23 account for each element E of urine

The urine mass flow, in dry weight, is:

$$W_{urine} = G_{SU,CC} \cdot M_{SU} + G_{H2SO4,CC} \cdot M_{H2SO4} + G_{H3PO4,CC} \cdot M_{H3PO4} \quad \text{(V.22)}$$

The volumetric flow of this stream is the sum of each volumetric flow:

$$Q_{Lout\_urine} = Q(H2O)_{WC\_urine} + Q_{H2O,body} \cdot f_{H2O,urine} + \frac{W_{urine}}{1000} \quad \text{(V.23)}$$

The molar outflow of each urine compound is:

$$Z_{i,\ Lout\_urine} = G_{i,CC} \cdot f_{i,urine} \cdot \frac{M_{SU}}{M_i} \quad \text{(V.24)}$$

→ For i = urea, cre, urid

For sulphate (H2SO4), phosphate (H3PO4) and water (H2O) is used equations V.25, V.26 and V.27 respectively.

$$Z_{H2SO4,Lout\_urine} = G_{H2SO4,CC} \quad \text{(V.25)}$$

$$Z_{H3PO4,Lout\_urine} = G_{H3PO4,CC} \quad \text{(V.26)}$$

$$Z_{H2O,Lout\_urine} = \frac{Q_{H2O,body} \cdot f_{H2O,urine}}{M_{H2O}} + \frac{Q(H2O)_{WC\_urine} \cdot 1000}{M_{H2O}} \quad \text{(V.27)}$$

The concentration of each urine compound is:

$$c_{i,Lout\_urine} = \frac{Z_{i,Lout\_urine}}{Q_{Lout\_urine}} \quad \text{(V.28)}$$

3.7.2.12 G_out (gas)

The gas collected from the crew chamber is the exhaled gas from the astronauts and contains CO_2. This stream also contains the expired and perspired water $Q_{H2O,Gout,}$, as volume per unit time, which is expressed through equation V.29. This equation takes into account the water vapour that the gas input contains.

$$Q_{H2O,Gout} = \frac{Q_{Gin} \cdot c_{H2O,Gin}}{1000} \cdot M_{H2O} + (f_{H2O,resp} + f_{H2O,persp}) \cdot Q_{H2O,body} \quad \text{(V.29)}$$

The molar inflow of each compound can be determined by V.30. In the gas stream none of these compounds, except oxygen and carbon dioxide, experience any change in the mol number, therefore, the molar gas inflow is equal to the outflow (see equation V.31). Additionally the generation term must be taken into account for O_2 and CO_2 (see equation V.32). For H_2O the volumetric flow in the gas phase is used (see equation V.33).

$$Z_{i,Gin} = Q_{i,Gin} \cdot c_{i,Gin} \quad \text{(V.30)}$$

→ for each compound “i”

$$Z_{i,Gout} = Z_{i,Gin} \quad \text{(V.31)}$$

→ for each compound “i” except for CO_2, O_2 and H_2O

$$Z_{i,Gout} = Z_{i,Gin} + G_{i,CC} \quad \text{(V.32)}$$

→ for the compounds i = CO_2, O_2

$$Z_{H2O,Gout} = \frac{Q_{H2O,Gout}}{M_{H2O}} \cdot 1000 \quad \text{(V.33)}$$

The volumetric flow of this stream can be expressed through the ideal gas equation:

$$Q_{Gout} = \frac{R \cdot T \cdot \sum Z_{i,Gout}}{Pr} \quad \text{(V.34)}$$

The concentration can be determined:

$$c_{i,Gout} = \frac{Z_{i,Gout}}{Q_{Gout}} \quad \text{(V.35)}$$

→ for each compound “i”

3.7.2.13 Lout_re stream (residual water)

This stream is composed of residual water from the crew cleanliness. Therefore, the volumetric flow is:

$$Q_{Lout\_re} = Q(H_2O)_{cl} \quad \text{(V.36)}$$

3.8 Other subsystems

3.8.1 Food Treatment Unit

3.8.1.1 Description

This unit represents every process that participates in supplying food for the crew. It receives the biomass from the higher plant chamber and from Compartment IVa. Furthermore it receives a certain quantity of biomass from outside the MELiSSA loop that offers the nutrients and the vitamins that the food from the loop cannot offer (see Figure 3-13).

For the food preparation the separation of the non-eatable parts of plants, which are sent to the Biomass Pre-treatment Unit (BPU) are included.

To summarize, the purpose of the mathematic model of this unit is to determine the additional biomass composition that must to be supplied from outside the loop. Therefore, an equilibrate diet for one person must be defined as baseline data. The steps for the solution are:

1. Determine the food characteristics (composition) from the MELiSSA loop destined for the crew
2. Determine the additional food characteristics (composition) from outside the loop
3. Calculate the quantity of non-eatable plants

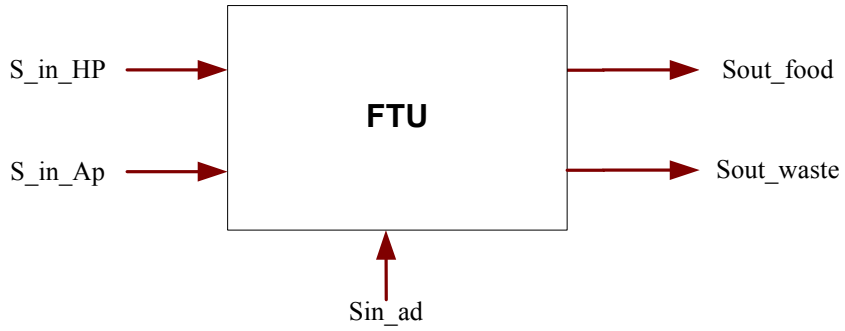


Figure 3-13: Food Treatment Unit

3.8.1.2 Assumptions

- The food composition destined towards the crew is given by a equilibrated diet

3.8.1.3 Operational Data

Parameters	Description	Value	Units
$(CHONSP)_{m,food}$	Composition of the macromolecules "m" of the food (in dry weight)	TBD	-

$f_{H2O,\,food}$	Mass fraction of water on the damp food	0,5 – 0,95	-
$f_{m,\,food}$	Macromolecular mass fraction of "m" on the dry food	TBD	-
n	Number of crew members	4	-
$W_{food,\,indiv}$	Mass flow of food for one person (in dry weight)	TBD	kg/s

Table 3-41: Data about food composition for one person

Note:
The sub-index “m” (in Table 3-41) represents the main biological macromolecule of the food: carbohydrates, proteins and lipids.

3.8.1.4 Food Characteristics

The objectives in this section in regard to the food are the followings:

1. Calculate the total mass flow destined towards the crew
2. Calculate water flow within
3. Calculate its CHONSP composition

By knowing the food mass flow required for one person and the number of astronauts, the total mass flow of food can be expressed:

$$W_{food} = W_{food,\,indiv} \cdot n \qquad \text{(FTU.1)}$$

The quantity of water that the total food contains is:

$$W_{H2O,\,food} = \frac{W_{food}}{1 - f_{H2O,\,food}} \cdot f_{H2O,\,food} \qquad \text{(FTU.2)}$$

The expression to obtain the CHONSP composition (equations UTC.3 and UTC.4) follows the same procedure then previous cases.

$$E_{food\_1} = \sum_{m} E_{m,\,food} \cdot \frac{f_{m,\,food}}{M_{m,food}} \qquad \text{(FTU.3)}$$

$$E_{food} = \frac{E_{food\_1}}{C_{food\_1}} \qquad \text{(FTU.4)}$$

→ Both equations FTU.3 and FTU.4 account for each element E.

3.8.1.5 Food Supply Characteristics

The additional food is the food supply that completes an equilibrated diet for the crew.

The objectives in this section, with regard to the food supply, are the followings:

1. Calculate its CHONSP composition
2. Calculate the mass fraction of the main macromolecules it is composed of
3. Calculate the CHONSP of the macromolecules it is composed of
4. Calculate its mass fraction of water

The food’s molar flow, Z_{food} can be determined since its mass flow and its molecular weight have been obtained before. Equally the *Arthrospira* and the comestibles higher plants molar flows, Z_{Ap} and Z_{HPc}, can be determined. Therefore, the CHONSP composition of the additional food can be calculated:

$$E_{adF\_1} = E_{food} \cdot Z_{food} - (E_{Ap} \cdot Z_{Ap} + E_{HPc} \cdot Z_{HPc}) - \sum_i (E_{i,Ap} \cdot Z_{i,Ap}) \quad \text{(FTU.5)}$$

$$E_{adF} = \frac{E_{adF\_1}}{C_{adF\_1}} \quad \text{(FTU.6)}$$

→ FTU.5 and FTU.6 account for each element E

The expression $\sum_i (E_{i,Ap} \cdot Z_{i,Ap})$ represents the total number of moles of the element E due to the compounds "i" that are in solution with *Arthrospira*.

The additional food mass flow, W_{adF}, is:

$$W_{adF} = W_{food} - Z_{Ap} \cdot M_{Ap} - Z_{HPc} \cdot M_{HPc} - \sum_i (Z_{i,Ap} \cdot M_i) \quad \text{(FTU.7)}$$

To obtain the macromolecules mass fraction of the additional food it is necessary to calculate the mass flows first:

$$W_{m,a} = f_{m,a} \cdot Z_a \cdot M_a \quad \text{(FTU.8)}$$

→ for each macromolecule "m" of each edible biomass "a", where

$m \in \{ch, lip, prot\}$ and $a \in \{Ap, HPc, food\}$

$$W_{m,adF} = W_{m,food} - W_{m,Ap} - W_{m,HPc} \quad \text{(FTU.9)}$$

→ for each macromolecule "m"

Thus, the mass fraction of each macromolecule in additional food is:

$$f_{m,adF} = \frac{W_{m,\ adF}}{W_{adF}} \quad \text{(FTU.10)}$$

→ for each macromolecule "m"

It is also necessary to calculate the CHONSP composition of each biological macromolecule of the additional food:

$$E_{m,adF\_1} = E_{m,food} \cdot Z_{food} - (E_{m,Ap} \cdot Z_{Ap} + E_{m,HPc} \cdot Z_{HPc}) \quad \text{(FTU.11)}$$

$$E_{m,adF} = \frac{E_{m,\ adF\_1}}{C_{m,adF\_1}} \quad \text{(FTU.12)}$$

→ for each element E of each macromolecule "m"

At last, it is necessary to know the mass fraction of water that the additional biomass must contain (equation FTU.14). That can be obtained by calculating the quantity of water required in the additional food (equation FTU.13)

$$W_{H2O,\ adF} = W_{H2O,\ food} - \frac{Z_{Ap} \cdot M_{Ap}}{1 - f_{H2O,Ap}} \cdot f_{H2O,Ap} - W_{H2O,\ HPc} \quad \text{(FTU.13)}$$

→ $\frac{Z_{Ap} \cdot M_{Ap}}{1 - f_{H2O,Ap}} \cdot f_{H2O,Ap}$ and $W_{H2O,\ HPc}$ are the quantity of water (per time unit) contained in the damp biomass of the Ap and HPc.

$$f_{H2O,adF} = \frac{W_{H2O,\ adF}}{W_{adF} + W_{H2O,adF}} \qquad \text{(FTU.14)}$$

3.8.1.6 Separation between inedible and edible parts of Higher Plants

Plants have parts that are not comestible for humans and its quantity depends on each vegetal species. This quantity is calculated in the Higher Plants Chamber (HPC), therefore, it is only necessary to define a volumetric flow that consist of the non-edible part and taking the water into account that this biomass contains.

$$Q_{Sout\_BPU} = \frac{W_{H2O,HPre} + W_{HPre}}{1000} \qquad \text{(FTU.15)}$$

→ In this equation it is assumed that the biomass has the same density than water

The concentration of the dry biomass in this stream is calculated through FTU.16 and the water concentration through FTU.17.

$$c_{HPre,Sout\_BPU} = \frac{\frac{W_{HPre}}{M_{HPre}}}{Q_{Sout\_BPU}} \qquad \text{(FTU.16)}$$

$$c_{H2O,Sout\_BPU} = \frac{\frac{W_{H2O,HPre}}{M_{H2O}}}{Q_{Sout\_BPU}} \qquad \text{(FTU.17)}$$

3.8.2 Liquid Collector and Distributor (LCD)

3.8.2.1 Description

The LCD represents the processes of liquid collection and distribution. On the one hand the liquid received from the compartments IVa and IVb is distributed to Compartment I, on the other hand the potable and hygiene water received from the WTU is distributed to the crew compartment and the Arthrospira Washing (AW). Furthermore, there is an additional water input if required.

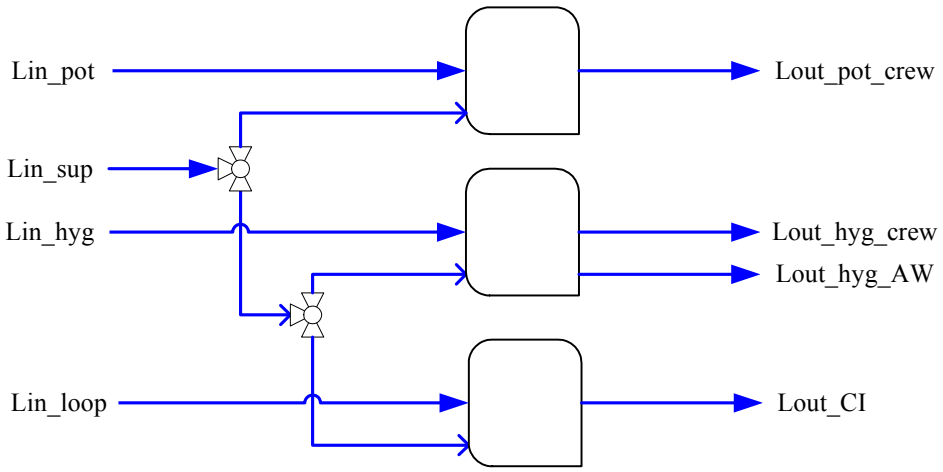


Figure 3-14: Liquid Collector and Distributor

The mathematic model calculates the quantity of additional water (Lin_sup in the figure) required, which will be solved in the following steps:

1. Determine the potable and hygiene water flows destined for the crew
2. Determine the liquid flow required for Compartment I
3. Determine the hygiene water needed for the AW.
4. Calculate the additional flows of:
    a. Potable water
    b. Hygiene water
    c. Water destined for Compartment I

3.8.2.2 Operational Data

Symbol	Description	Value	Units
n	Number of crew members	4	-
$Q_{hyg,\ WA}$	Volumetric Flow of hygienic water required for AW	TBD	m^3/s
$Q^{indiv}_{hyg,CC}$	Volumetric flow of hygiene water per person	TBD	m^3/s
$Q_{L,CI}$	Volumetric Flow of liquid required for BR_CI	TBD	m^3/s
$Q^{indiv}_{pot,CC}$	Volumetric flow of potable water per person	TBD	m^3/s

Table 3-42: Operational data for the LCD

3.8.2.3 Water for the Crew Chamber

The volume of hygiene and potable water per time unit required for one person is given in the operational data (Table 3-42). The volumetric flows of potable and hygiene water for all crew members are obtained through the equations LCD.1 and LCD.2.

$$Q_{Lout\_pot} = n \cdot Q^{indiv}_{pot,CC} \qquad \text{(LCD. 1)}$$

$$Q_{Lout\_hyg} = n \cdot Q^{indiv}_{hig,CC} \qquad \text{(LCD.2)}$$

3.8.2.4 Liquid stream for Compartment I and for Arthrospira Washer (AW)

To determine the flows for CI and for AW calculations are not necessary, as both are operational data:

$Q_{Lout\_CI} = Q_{hyg,CI}$ and $Q_{Lout\_AW} = Q_{hyg,AW}$

The stream going to the AW has to be pure water, free of any compounds.

The stream for Compartment I is composed of the compounds that have been re-circulated, with a concentration of:

$$c_{i,Lout\_CI} = \frac{c_{i,Lin\_loop} \cdot Q_{Lin\_loop}}{Q_{Lout\_CI}} \qquad \text{(LCD.3)}$$

→ for each compound “i” except for H2O. For H2O it is:

$$c_{H2O,Lout\_CI} = \frac{Z_{H2O\_CI,ad} + c_{Lin\_loop} \cdot Q_{Lin\_loop}}{Q_{Lout\_CI}}$$

→ Where $Z_{H2O\_CI,ad}$ is the additional molar flow of water for CI

3.8.2.5 Additional Water (Water Supply)

Additional potable and hygiene water is needed and can be calculated as follows:

a. Additional potable water for the crew

$$Q_{pot,\ ad} = Q_{Lout,\_pot} - Q_{Lin,\_pot} \qquad \text{(LCD.4)}$$

b. Additional hygiene water for the crew and for the AW

$$Q_{hyg,\ ad} = Q_{Lout\_hyg} + Q_{Lout\_AW} - Q_{Lin\_hyg} \qquad \text{(LCD.5)}$$

c. Additional hygiene water for Compartment I

$$Q_{H2O\_CI,\ ad} = Q_{Lout\_CI} - Q_{Lin\_loop} \qquad \text{(LCD.6)}$$

The total additional water is the sum of the three flows (equation LCD.7), that can be supplied separately or as one stream of potable water.

$$Q_{Lin\_sup} = Q_{pot,ad} + Q_{hyg,ad} + Q_{H2O\_CI,\ ad} \qquad \text{(LCD.7)}$$

3.8.3 Biomass Pre-treatment Unit (BPU)

3.8.3.1 Description

In the BPU all biomasses are collected, mixed with water and undergo a physic-mechanical pre-treatment of the biomass to support the anaerobic degradation in the BR_CI in which the biomass is send in form of a liquid stream (see Figure 3-15).

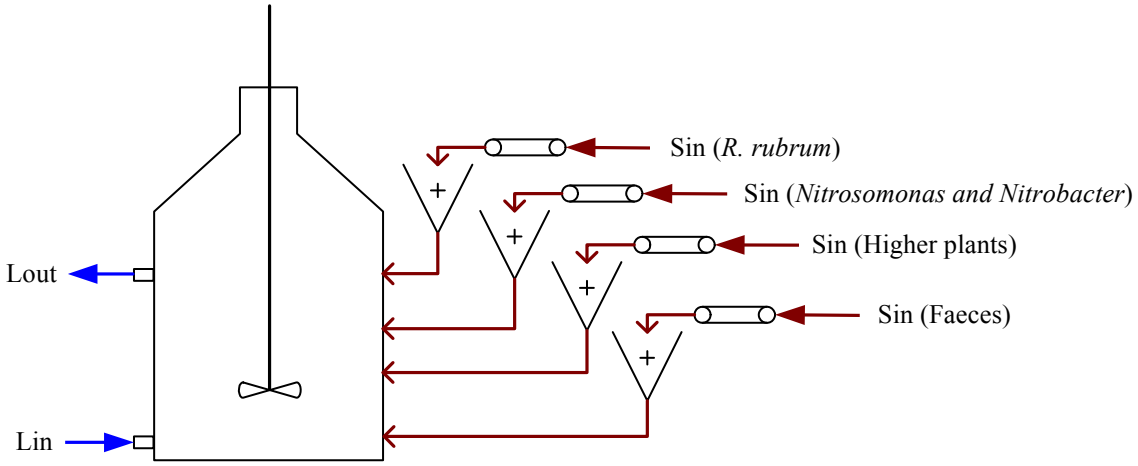


Figure 3-15: Biomass Pre-treatment Unit

The main purpose of the pre-treatment is the particle size reduction, which produces an increase in the hydrolysis rate. As the hydrolysis is the limiting stage of the anaerobic process, the pre-treatment supports the general process by producing smaller retention times and leads to a smaller reactor size. There are different pre-treatment processes existing, using ultrasounds, mechanics, thermals, etc.

The mathematic model applied for the BPU is only representing mathematically the biomasses mix, which is expressed as only one mass called Residual Biomass (RB) containing a CHONSP composition resulted from the mix:

$$[CHONSP]_{R.\,rubrum} + [CHONSP]_{Nitrosomonas\ -\ Nitrobacter} + [CHONSP]_{HPS\,residual} + [CHONSP]_{faeces}$$

$$\Downarrow$$

$$[CHONSP]_{Residual\,Biomass}$$

Thus, the mathematic model objective is to determine the volumetric flow of the outlet stream and its composition. The steps for the solution are the following:

1. Calculate the CHONSP composition of the Residual Biomass as well as its mass flow and the quantity of proteins, lipids and carbohydrates contained.
2. Calculate the volumetric flow and the concentration at the outlet.

3.8.3.2 Residual Biomass Composition

The CHONSP composition, the molecular weight and the mass flows of each biomass entering the BPU are calculated in the correspondent subsystem. The CHONSP composition of the final residual biomass can be determined by equation BPU.1 and BPU.2.

$$E_{RB\_1} = \sum_b E_b \cdot Z_{b,in} \qquad \text{(BPU. 1)}$$

→ $b \in \{Rr, fc, New, HPre\}$

$$E_{RB} = \frac{E_{RB\_1}}{C_{RB\_1}} \qquad \text{(BPU. 2)}$$

→ BPU.1 and BPU.2 account for each element E.

The Residual Biomass flow is:

$$W_{RB,Lout} = \sum_b Z_{b,in} \cdot M_b \qquad \text{(BPU. 3)}$$

→ With:

$Z_{b,in}$ = Molar inflow of the biomass “b” (mol/s)

M_b = Molecular Weight of the biomass “b” (kg/mol)

The mass fraction of the proteins, lipids and carbohydrates in the residual biomass can be calculated through the respective fractions in each biomass (equation BPU.4).

$$f_{m,RB} = \frac{\sum_b f_{m,b} \cdot M_b \cdot Z_{b,in}}{W_{RB,Lout}} \qquad \text{(BPU. 4)}$$

→ Equation for each macromolecule “m”

The mass flow of water contained in each biomass is:

$$W_{H2O,b} = \frac{Z_{b,in} \cdot M_b}{1 - f_{H2O,b}} \cdot f_{H2O,b} \qquad \text{(BPU. 5)}$$

→ Equation for each biomass b

The quantity of water contained in the residual biomass is the addition of the water contained in each biomass. It is composed of all biomasses:

$$W_{H2O,RB} = \sum_b W_{H2O,b} \qquad \text{(BPU. 6)}$$

The mass fraction of water in the damp residual biomass is:

$$f_{H2O,RB} = \frac{W_{H2O,RB}}{W_{H2O,RB} + W_{RB,Lout}} \qquad \text{(BPU. 7)}$$

3.8.3.3 Liquid Stream Outlet

The volumetric outflow, Q_{Lout}, is the sum of the volumetric inflows.

The residual biomass concentration is:

$$c_{RB,Lout} = \frac{Z_{RB,Lout}}{Q_{Lout}} \quad \text{(BPU. 8)}$$

→ With:

$$Z_{RB,Lout} = \frac{W_{RB,Lout}}{M_{RB}} \quad \text{(BPU. 9)}$$

For the remaining compounds the inflows have been taken into account:

$$c_{i,\ Lout} = \frac{c_{i,Lin} \cdot Q_{Lin} + c_{i,Sin\_Rr} \cdot Q_{Sin\_Rr} + c_{i,Sin\_New} \cdot Q_{Sin\_New} + c_{i,Sin\_New} \cdot Q_{Sin\_New} + c_{i,Sin\_fc} \cdot Q_{Sin\_fc}}{Q_{Lout}} \quad \text{(BPU. 10)}$$

→ BPU.10 accounts for each compound "i" except for the biomasses, as it is defined as one biomass, the residual biomass.

3.8.4 Solid-Liquid Separator (SLS)

3.8.4.1 Description

This subsystem represents the processes of solid-liquid separation, to precipitate the biomass particles from the liquid stream (see Figure 3-16), for example by the use of a filtration unit linked with a centrifugation system. The separated biomass is sent to the Solid Distributor, while the liquid flows to the next compartment.

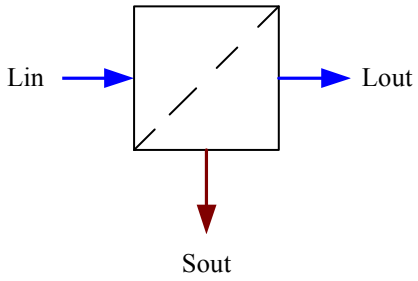


Figure 3-16: Solid-Liquid Separator

After the biomass has been extracted from the liquid, the concentration of each compound in this liquid is modified. To distinguish between liquid with biomass, called "liquid" and liquid without biomass called "dissolution" (see Figure 3-17), the compounds in the dissolution are dissolved and are called "Solute". Therefore, the stream Lin in Figure 3-16 is composed of the liquid; the stream Sout is composed of the solid (biomass + dissolution) and the stream Lout is composed of the dissolution. It is important to note that the composition of the dissolution is the same in the inlet than in the outlet while the biomass has varying quantities.

Furthermore, the biomass is measured in dry weight, even though in reality a great part of it is composed of water. Consequently the water contained in the biomass has been taken into account separately for the calculations (data given in each compartment, as $f_{H2O,bio}$).

MELiSSA needs four SLS, which have the same mathematic model under the assumption of a complete separation of all biomass from the liquid. Nevertheless, each SLS can represent

different processes of separation. The quantity of dissolution gained from the biomass, depends on treatment method and its efficiency, which is an operational data.

The objective is to obtain the new outlet concentrations and the volumetric flows in both the solid stream and the liquid stream. The steps for the solution are:

1. Calculate the liquid density in the inlet
2. Calculate the biomass density
3. Calculate the volumetric outflows:
    a. Sout (biomass + dissolution)
    b. Lout (liquid without biomass, dissolution)
4. Calculate the concentration of each compound in both outlets:
    a. Lout (liquid without biomass, dissolution)
    b. Sout (biomass + dissolution)

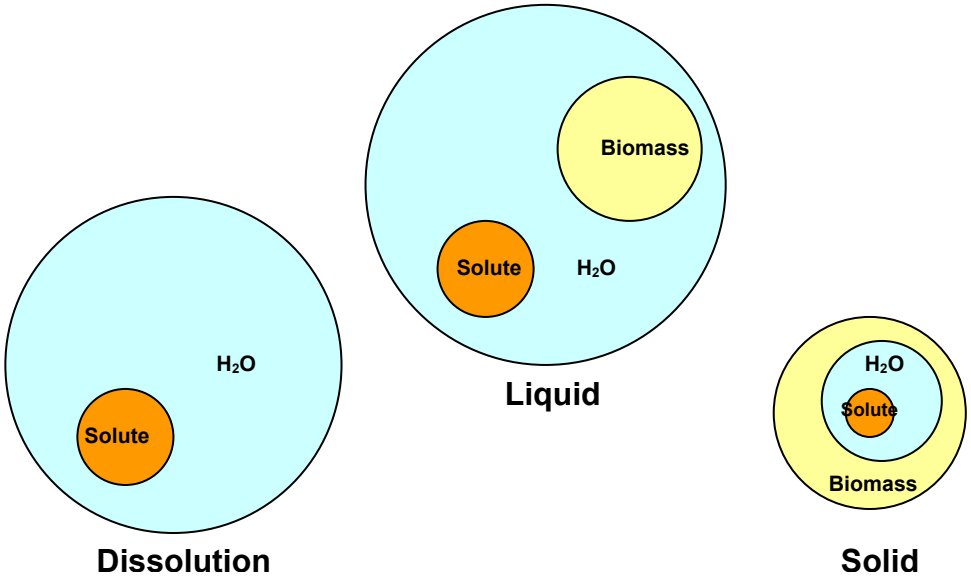


Figure 3-17: Definition of Liquid, Dissolution and Solid

3.8.4.2 Operational Data

Symbol	Description	Units
$f_{don,bio}$	Mass fraction of dissolution in the solid flow; the dissolution of kilograms of biomass out of each kilogram of damp biomass	-
pH	pH concentration of the respective compartment	-
T	Temperature of the respective compartment	K
ρ_{don}	Density of the dissolution. As an approximation it is considered equal to the density of water (1000).	$(kg)_{don}/(m^3)_{don}$

Table 3-43: Operational Data of SLS

3.8.4.3 Liquid Density

As has been explained, the liquid stream that enters to the SLS contains the dissolution and the biomass. The liquid density is:

$$\rho_L = \sum_i (c_{i,Lin} \cdot M_i) \qquad \text{(SLS. 1)}$$

→ "i" belongs to all the compounds

3.8.4.4 Biomass Density

To calculate the biomass density the following steps are necessary:

A. Calculation of the Mass Flows in the Inlet Stream: Lin

The mass flows of each compound "i" can be determined (equation SSL.2) and, consequently, the total mass flow, the damp biomass flow (equation SLS.4) and the dissolution mass flow (equation SLS.5):

$$W_{i,Lin} = Q_{Lin} \cdot c_{i,Lin} \cdot M_i \qquad \text{(SLS. 2)}$$

→ Equation for each compound "i"

$$W_{Lin} = \sum_i W_{i,Lin} \qquad \text{(SLS. 3)}$$

→ "i" belongs to all the compounds

$$W_{damp\_bio,Lin} = \frac{W_{dry\_bio}}{1 - f_{H2O,bio}} \qquad \text{(SLS. 4)}$$

→ The sub-index "damp_bio" represents the biomass with its own water. The sub-index "dry_bio" represents the dry biomass, without taking into account the water. Depending on each SLS, this biomass can be: *Arthrospira platensis* (Ap), *R. rubrum* (Rr), faeces (fc) and *Nitrosomonas* and *Nitrobacters* (New).

$$W_{don,Lin} = W_{Lin} - W_{damp\_bio,Lin} \qquad \text{(SLS. 5)}$$

B. Calculation of the Density Biomass

Assuming the value of the dissolution density (given in the operational data), the biomass density can be determined:

$$\rho_{bio} = \frac{\frac{W_{damp\_bio,Lin}}{Q_{Lin}}}{1 - \frac{\frac{W_{don,Lin}}{Q_{Lin}}}{\rho_{don}}} \qquad \text{(SLS. 6)}$$

3.8.4.5 Volumetric Flows

a. Sout Stream:

The Sout stream consists of the biomass and its connected dissolution. The quantity of its dissolution is determined through the operational data $f_{don,bio}$. Through the densities, the volumetric flows can be obtained:

$$Q_{Sout} = \frac{W_{damp\_bio,Lin}}{\rho_{bio}} + \frac{W_{damp\_bio,Lin} \cdot f_{don,\ bio}}{\rho_{don}} \qquad \text{(SLS. 7)}$$

b. Lout Stream:

In the SLS the volume is additive, therefore, the volumetric flow of this stream is:

$$Q_{Lout} = Q_{Lin} - Q_{Sout} \quad \text{(SLS. 8)}$$

3.8.4.6 Concentration of each compound in each outlet stream

The compound's concentration in the dissolution is:

$$c_{i,don} = \frac{c_{i,Lin} \cdot \rho_{don}}{\rho_L - \frac{W_{damp\_bio,Lin}}{Q_{Lin}}} \quad \text{(SLS. 9)}$$

→ for each compound "i" that belongs to the solute. That means all compounds "i" except the solvent water and the biomass.

a. Lout Stream:

The Lout stream contains the dissolution, thus the concentration for each compound is:

$$c_{i,Lout} = c_{i,don} \quad \text{(SLS. 10)}$$

→ For each compound "i" from the solute

The concentration of the biomass in this stream is zero. For water, H2O, the concentration is:

$$c_{H2O,Lout} = \frac{\rho_{don} - \sum_i c_{i,Lout} \cdot M_i}{M_{H2O}} \quad \text{(SLS. 11)}$$

The ions concentration and the pure concentration depend on the pH and on the T and are determined through the equations 8 and 9.

b. S2 Stream:

The concentration for each compound, except for water and biomass, are calculated through SLS.12:

$$c_{i,Sout} = \frac{c_{i,don} \cdot \frac{W_{damp\_bio,L1} \cdot f_{don,\ bio}}{\rho_{don}}}{Q_{Sout}} \quad \text{(SLS. 12)}$$

→ For each compound "i" from the solute

The dry biomass concentration is:

$$c_{dry\_bio,\ Sout} = \frac{c_{dry\_bio,\ Lin} \cdot Q_{Lin}}{Q_{Sout}} \quad \text{(SLS. 13)}$$

To obtain the water concentration, both the water medium (the solvent) and the water contained in the biomass have been taken into account:

$$c_{H2O,Sout} = \frac{(W_{damp\_bio,Lin} \cdot f_{don,bio} - \sum_i c_{i,Sout} \cdot M_i \cdot Q_{Sout}) + W_{damp\_bio,Lin} \cdot f_{H2O,bio}}{M_{H2O} \cdot Q_{Sout}} \quad \text{(SLS. 14)}$$

3.8.5 Atmosphere Generator (AG)

3.8.5.1 Description

The AG represents the preparation of breathable atmosphere for the crew at the required pressure and temperature (see Figure 3-18).

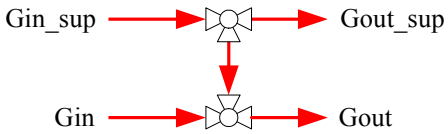


Figure 3-18: Atmosphere Generator

The objective of the mathematic model is to obtain the necessary molar flow of nitrogen to achieve the crew requirements.

3.8.5.2 Operational Data

Symbol	Description	Units
$H_{N2,O2}$	Relationship between moles of nitrogen and oxygen in the atmosphere of the CC	-
Pr	Pressure required for the CC	Pa
R	Gas constant	J/(mol K)
T	Temperature required for the CC	K

Table 3-44: Operational Data for AG

3.8.5.3 Molar Inflows

The moles of each compound of the gas inlet stream are given by AG.1, while the moles of each compound of the supply inlet stream are given by AG.2:

$$Z_{i,Gin} = Q_{Gin} \cdot c_{i,Gin} \qquad \text{(AG. 1)}$$

$$Z_{i,Gin\_sup} = Q_{Gin\_sup} \cdot c_{i,Gin\_sup} \qquad \text{(AG. 2)}$$

→ Both equations account for each compound “i”

3.8.5.4 Nitrogen Requirements

The molar outflow of nitrogen at the gas stream for the crew must fulfil the crew requirements. This flow is calculated through equation AG.3. To achieve this quantity additional nitrogen has to be considered (equation AG.4).

$$Z_{N2,Gout} = Z_{O2,Gout} \cdot H_{N2,O2} \qquad \text{(AG. 3)}$$

$$Z_{N2,ad} = Z_{N2,Gin} - Z_{N2,Gout} \qquad \text{(AG. 4)}$$

The volumetric flow of additional nitrogen is:

$$Q_{ad} = \frac{Z_{N2,ad}}{c_{N2,Gin\_sup}} \qquad \text{(AG. 5)}$$

3.8.5.5 Molar Outflows. Balances

The molar flow of each compound at the outlet gas stream takes the additional flow into account:

$$Z_{i,Gout} = Z_{i,Gin} + Q_{ad} \cdot c_{i,Gin\_sup} \qquad \text{(AG. 6)}$$

→ For each compound "i"

The molar flow of each compound at the supply outlet gas stream is the subtraction of the supply flow from the supply molar inflow:

$$Z_{i,Gout\_sup} = Z_{i,Gin\_sup} - Q_{ad} \cdot c_{i,Gin\_sup} \qquad \text{(AG. 7)}$$

→ For each compound "i"

3.8.5.6 Volumetric Outflows and Concentrations

Gas Outlet Stream (Gout)

This stream of atmosphere gas fulfils the crew requirements. The volumetric flow is a function of the molar flows of each compound "i" as well as of the temperature and the pressure required for the crew compartment.

$$Q_{Gout} = \frac{\sum_i Z_{i,Gout}}{Pr} \cdot R \cdot T \qquad \text{(AG. 8)}$$

The concentration at this stream is:

$$c_{i,Gout} = \frac{Z_{i,Gout}}{Q_{Gout}} \qquad \text{(AG. 9)}$$

→ For each compound "i"

Gas Supply Outlet Stream (Gout_sup)

This stream contains the unused nitrogen gas. The volumetric flow is the subtraction of the additional volumetric supply flow from the volumetric inflow.

$$Q_{Gout\_sup} = Q_{Gin\_sup} - Q_{ad} \qquad \text{(AG. 10)}$$

The concentrations at this stream remain constants.

3.8.6 Distributors (GD, LD and SD)

3.8.6.1 Description

The distributor (Figure 3-19) represents a valve with the function to distribute the inflow.

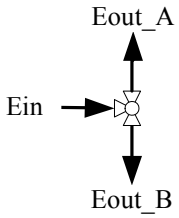


Figure 3-19: Distributor

In MELiSSA there are three Gas Distributors (GD) one Liquid Distributor (LG) and five Solid Distributors (SD). Amongst the GDs, there is one to distribute the outflow from the CI to CII and CDC (Carbon Dioxide Collector), another from the CDC outlet to the two photosynthetic compartments, and one to distribute the atmosphere gas between the CC and the BR_CIII.

The LG receives the filtered liquid from the nitrifying bioreactor in order to distribute it between the two photosynthetic compartments.

The five SD are one for each biomass:

- *Arthrospira*
- *R. rubrum*,
- *Nitrosomonas* and *Nitrobacter*,
- Non-edible parts of higher plants
- faeces

All three distributor types follow the same mathematic model, with the objective to determine the volumetric outflows.

3.8.6.2 Operational Data

Symbol	Description	Units
D	Distribution Coefficient; the relationship between outflow and inflow	-

Table 3-45: Operational Data of Distributor

3.8.6.3 Volumetric Outflows

For a distributor as shown in Figure 3-19, the volumetric outflows, Q_{Eout_A} and Q_{Eout_B}, are given below, with the volumetric inflow Q_{Ein}:

$$Q_{Eout\_A} = Q_{Ein} \cdot D \quad \text{(D.1)}$$

$$Q_{Eout\_B} = Q_{Ein} - Q_{Eout\_A} \quad \text{(D.2)}$$

In all three streams the concentration of each compound is the same.

3.8.7 Collectors (CDC, MOC, LC)

3.8.7.1 Description

There are three different collectors: the Carbon Dioxide Collector (CDC), the Molecular Oxygen Collector (MOC) and the Liquid Collector (LC). Each of them represents the collection of different streams to merge them into one. For carbon dioxide rich gas streams the CDC is used, for oxygen rich gas streams the MOC is used and for liquid streams the LC is used (see Figure 3-20).

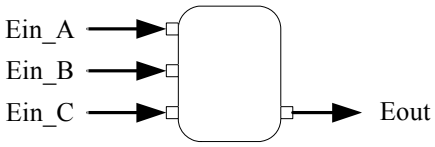


Figure 3-20: Collector

For each collector the applied mathematic model is the same, in which the concentration of each compound and the volumetric flow of the resulting stream are obtained.

3.8.7.2 Volumetric Outflows and Concentrations

Each collector has more then one inlet and one outlet only. The volume is additive because there are not chemical reactions or phase changes (see equation C.1):

$$Q_{Eout} = Q_{Ein\_A} + Q_{Ein\_B} + Q_{Ein\_C} \quad \text{(C. 1)}$$

The total molar outflow of each compound is also the sum of the molar inflows:

$$Z_{i,\,Eout} = Z_{i,\,Ein\_A} + Z_{i,\,Ein\_B} + Z_{i,\,Ein\_C} \quad \text{(C. 2)}$$

Thus, the concentration of each compound can be calculated:

$$c_{i,\,Eout} = \frac{Z_{i,\,Eout}}{Q_{Eout}} \quad \text{(C. 3)}$$

→ C.2 and C.3 account for each compound “i”

3.8.8 Condenser (C_HPC)

3.8.8.1 Description

This subsystem represents the condensation of the water transpired by the higher plants (see Figure 3-19).

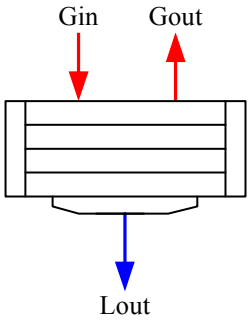


Figure 3-21: Condenser

It is assumed that the temperature for the condensation is adjusted to result only in water condensation.

Through the equations the concentration of each compound in the resulting gas, the volumetric outflow and the quantity of condensed water can be obtained.

3.8.8.2 Operational Data

Symbols	Description	Units
Pr	Pressure	Pa
R	Gas constant	J/(Pa mol)
T	Operation temperature – in a temperature range where only water condenses	K

Table 3-46: Operational Data of Condenser

3.8.8.3 Water Condensed

The steps for the calculation are:

A. Calculate the molar fraction of water in the gas inflow ($h_{H2O,Gin}$)

$$h_{H2O,Gin} = \frac{Z_{H2O,Gin}}{Z_{Gin}} \quad \text{(C_HPC 1)}$$

→ Z_{Gin} is the total molar flow of the Gin stream (mol/s)

→$Z_{H2O,Gin}$ is the molar flow of water (mol/s)

B. Calculate the molar fraction in saturation conditions

$$h_{H2O,sat} = \frac{P_{sat,H2O}}{Pr} \quad \text{(C_HPC 2)}$$

→ With $P_{sat,H2O}$ being the saturation pressure of water and a function of temperature. It can be calculated through a function that is implemented in EcosimPro®.

C. Determine the molar flow of condensate water and the volumetric flow

$$Z_{H2O,cond} = (H_{H2O,Gin} - H_{H2O,sat}) \cdot (Z_{Gin} - Z_{H2O,Gin}) \quad \text{(C_HPC 3)}$$

→ With:

$$H_{H2O,Gin} = \frac{h_{H2O,Gin}}{1 - h_{H2O,Gin}} \quad \text{(C_HPC 4)}$$

$$H_{H2O,sat} = \frac{h_{H2O,sat}}{1 - h_{H2O,sat}} \quad \text{(C_HPC 5)}$$

$$Q_{H2O\_cond} = \frac{Z_{H2O,cond} \cdot M_{H2O}}{1000} = Q_{Lout} \quad \text{(C_HPC 6)}$$

3.8.8.4 Gas Outflow

The molar flow of the water that does not condensate and, therefore, keeps in gas phase is:

$$Z_{H2O,Gout} = H_{H2O,sat} \cdot (Z_{Gin} - Z_{H2O,Gin}) \quad \text{(C_HPC 7)}$$

For the others compounds the molar flow keeps unchanged, as it is assumed that they do not condensate.

The volumetric outflow of the gas stream is calculated through the ideal gas equation (equation C_HPC.8) and therefore the concentration can be determined (equation C_HPC.9).

$$Q_{Gout} = \frac{\sum_{i} Z_{i,Gout} \cdot R \cdot T}{Pr} \qquad \text{(C\_HPC 8)}$$

$$c_{i,Gout} = \frac{Z_{i,Gout}}{Q_{Gout}} \qquad \text{(C\_HPC 9)}$$

3.8.9 Arthrospira Washing (AW)

3.8.9.1 Description

This subsystem is the representation of the *A. platensis* washing with the aim to eliminate the solute that (ammonia, nitrates, sulphates, phosphates, carbonates, etc.) accompanies this biomass. Thus, the algae will be appropriate to be eaten by the crew.

The mathematic model applied is based on a matter exchange between the two streams flowing in opposite directions, as shown in Figure 3-22, for n equilibrium stages. Hygiene water (without solute) enters the unit (Lin) and dissolves the solute of the dissolution of the Sin stream.

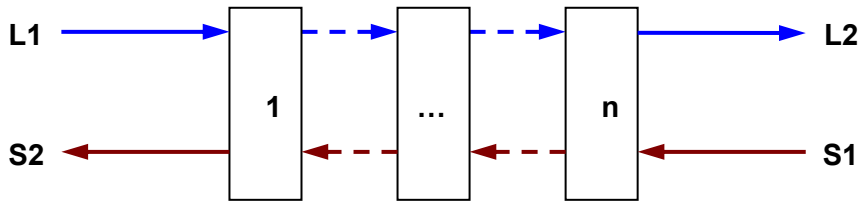


Figure 3-22: Arthrospira Washing

The mathematic model's objective is to obtain the volumetric flows and the concentrations in the outlet streams of the AW. Therefore, the mass balance for each equilibrium stage and the equilibrium equations must be used. It is assumed that the volumetric flows are constant for both streams, liquid and solid. Figure 3-23 shows the representation of an equilibrium stage.

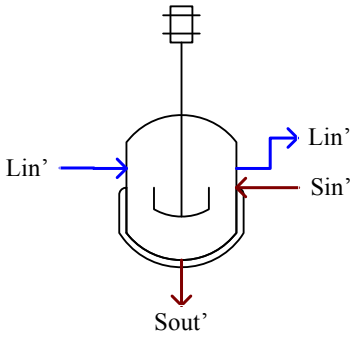


Figure 3-23: Equilibrium Stage

Thus, the system equation can be resolved, if the equilibrium stages (design condition) as well as the volumetric flow of hygiene water (Lin stream) are fixed.

In the following sections, the mathematic model is explained for one equilibrium stage and follows the steps presented below:

1. Calculate the biomass density
2. Calculate the molar fractions of the solute compounds
3. Calculate the solute concentration in the dissolution of the inlet streams
4. Calculate the volumetric flow of the dissolution of the Sin stream
5. Express the mass balance equations and equilibrium for the solute and the water
6. Calculate the volumetric flows and the concentrations in the outlet streams:
   a. Liquid (Lout)
   b. Solid (Sout)

3.8.9.2 Assumptions

- The volumetric flows are constants
- The solid stream that exits the AW contains the same quantity of dissolution then the solid stream of the inlet, since the biomass retains the same quantity.

3.8.9.3 Operational Data

Symbol	Description	Units
Pr	Operation pressure – same value as respective bioreactor	Pa
R	Gas constant	J/(Pa mol)
T	Operation temperature – same value as respective bioreactor	K
ρ_{don}	Density of the dissolution- to be considered equal to the water and constant throughout all stages of balance.	kg/m^3

Table 3-47: Operational Data of AW

3.8.9.4 Biomass density

The density of the damp *Arthrospira platensis* biomass is calculated in the same way then for the SLS (section 3.8.4.4).

3.8.9.5 Molar fraction of the solute compounds

The solute is composed of all compounds except of water which is the solvent and the biomass which is not dissolved. Thus, the molar flow of solute is the sum of the consisting compounds:

$$Z_{solute,Sin'} = \sum_{i} Z_{i,Sin'} \qquad \text{(AW. 1)}$$

→ "i" symbolizes all compounds except H2O and biomass

The molar fraction of each compound of the solute, $h_{i,solute}$, can be calculated through the equation AW.2 and expresses each compound's proportion and constant throughout the AW unit.

$$h_{i,solute} = \frac{Z_{i,Sin'}}{Z_{solute,Sin'}} \qquad \text{(AW. 2)}$$

→ For each compound "i", except H2O and biomass

3.8.9.6 Solute Concentration in the Dissolution of the Inlet Streams, Lin' and Sin''

The Lin' stream is only composed of dissolution; therefore, the solute concentration is the sum of each compound's concentration, which forms this dissolution (equation AW.3). The Sin' stream, however, is composed of both the dissolution and the biomass, but the concentration of the solute compounds, $c_{i,don,Sin'}$, must be referred to the volume of the dissolution (equation AW.5) before being summed up to obtain the solute concentration (equation AW.4).

$$c_{solute,Lin'} = \sum_i c_{i,Lin'} \qquad \text{(AW. 3)}$$

→ The sum accounts for each compound "i", except H2O and the biomass

$$c_{solute,don,Sin'} = \sum_i c_{i,don,Sin'} \qquad \text{(AW. 4)}$$

→ The sum accounts for each compound "i", except H2O and the biomass, with:

$$c_{i,don,Sin'} = \frac{c_{i,Sin} \cdot \rho_{don}}{\rho_L - \frac{W_{bio,Sin}}{Q_{Sin}}} \qquad \text{(AW. 5)}$$

→ for each compound "i", except for H2O and the biomass

A.1 Dissolution Volumetric Flow of the Sin Stream

Assuming the dissolution density is constant, the volumetric flow in the Sin' stream remains constant and its value is:

$$Q_{don,Sin'} = \frac{W_{don,Sin'}}{\rho_{don}} \qquad \text{(AW. 6)}$$

→ Where $W_{don,Sin'}$ is the dissolution mass flow

A.2 Mass Balance and Equilibrium

Considering the volumetric flows being constant, the mass balance for the solute in each stage is:

$$Q_{don,Sin'} \cdot (c_{solute,don,Sin'} - c_{solute,don,Sout'}) = Q_{Lin'} \cdot (c_{solute,Lout'} - c_{solute,Lin'}) \qquad \text{(AW. 7)}$$

The equilibrium equation expresses that the solute concentration in the dissolution of the solid outlet, Sout', is equal to the solute concentration in the liquid outlet, Lout'.

$$c_{solute,don,Sout'} = c_{solute,Lout'} \qquad \text{(AW. 8)}$$

Thus, the equation system is determined.

A.3 Outlet Stream Distribution

a. <u>Liquid Stream, Lout'</u>

Lout' stream is only composed of the dissolution; therefore the solute concentration is already determined with the mass balances and the equilibrium equations. The molar fraction is used to obtain the concentration of each compound of the solute:

$$c_{i,Lout'} = h_{i,solute} \cdot c_{solute,Lout'} \qquad \text{(AW. 9)}$$

→ for each compound "i", except H2O and Ap

The *A. platensis* biomass (Ap) stream is zero. For water (H2O) it is:

$$c_{H2O,Lout'} = \frac{\rho_{don} - \sum_i c_{i,Lout'} \cdot M_i}{M_{H2O}}$$

b. Solid Stream, Sout'

The biomass concentration is constant, because the solid volumetric flow has been considered constant and the biomass retains always the same quantity of dissolution.

The solute concentration in the Sout' stream is determined by AW.10 and the concentration of each compound of the solute is determined through the molar fraction (equation AW.11).

$$c_{solute,Sout'} = \frac{c_{solute,don,Sout'} \cdot Q_{don,Sin'}}{Q_{Sout'}} \quad \text{(AW. 10)}$$

$$c_{i,Sout'} = h_{i,solute} \cdot c_{solute,Sout'} \quad \text{(AW. 11)}$$

The water concentration in the dissolution of the Sout' stream increases in each stage because of the solute reduction. The water contained in *Arthrospira platensis* must also be taken into account.

$$c_{H2O,Sout'} = \frac{(Q_{don,Sin'} \cdot \rho_{don} - \sum_i c_{i,Sout'} \cdot M_i \cdot Q_{Sout'}) + W_{damp\_bio,Sin'} \cdot f_{H2O,Ap}}{M_{H2O} \cdot Q_{Sout'}} \quad \text{(AW. 12)}$$

3.8.10 Purge (P)

3.8.10.1 Description

The purge's function is to remove certain products from the system to avoid accumulation (Figure 3-24). Physically a purge can be exactly like a valve and mathematically behaves as a Distributor.

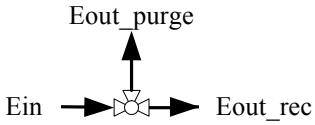


Figure 3-24: Purge

The objective of the mathematic model is to calculate the volumetric outflows. The equations are equal to the equations applied for distributors, considering that the inflow and one of the outflows are related by a coefficient. However, for the purge this coefficient is not an operational data but is an unknown.

3.8.10.2 Volumetric Outflows

"r" is the coefficient that relates one outflow with the inflow. The corresponding equations are:

$$Q_{Eout\_rec} = Q_{Ein} \cdot r \quad \text{(P.1)}$$

$$Q_{E2\_purge} = Q_{Ein} - Q_{Eout\_rec} \quad \text{(P.2)}$$

The concentrations remain constant throughout this subsystem.

3.8.11 Union Point (UP)

3.8.11.1 Description

The Union Point has the function to merge the flow from the system with the additional substance flow that is needed (objective compound) and added from outside (Figure 3-25)

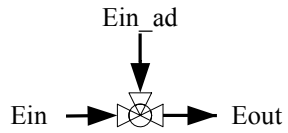


Figure 3-25: Union Point

The mathematic model objective is to obtain the additional flow, as well as the outflow of the Union Point. The equations vary depending on the stream being of liquids or gases. Through a gas stream pure compounds are added, while with a liquid stream substances dissolved in water with a known concentration are added.

3.8.11.2 Operational Data

Table 3-48 is for a UP with gas streams, while Table 3-49 is for a UP with liquid streams

Symbol	Description	Units
Pr	Pressure at the outflow	Pa
T	Temperature at the outflow	K

Table 3-48: Operational Data for a UP of gas streams

Symbol	Description	Units
$c_{i,ad}$	Concentration of the compounds in the additional dissolution	mol/m^3

Table 3-49: Operational Data for a UP of liquid streams

3.8.11.3 Flows and Concentrations

In this subsystem the molar flow of the objective compound is the only one that changes:

$$Z_{i,\,Ein} + Z_{i,\,Ein\_ad} = Z_{i,\,Eout} \qquad \text{(U. 1)}$$

→ for the compound objective "i". Z_{i,Ein_ad} is the molar flow of the compound necessary for the system.

To obtain the volumetric outflow from the UP the equations depend on the phase of the stream, as explained before.

UP of gas streams

In this case the volumetric outflow is calculated by the ideal gasses equation:

$$Q_{Eout} = \frac{\sum_i Z_{i,\,Eout}}{Pr} \cdot R \cdot T \qquad \text{(U. 2)}$$

UP of liquid flows

In this case the additional volumetric flow depends on the composition of the additional dissolution:

$$Q_{Eout} = Q_{Ein} + Q_{Ein\_ad} \qquad \text{(U. 3)}$$

→ With:

$$Q_{Ein\_ad} = \frac{Z_{i,\,Ein\_ad}}{c_{i,\,Ein\_ad}} \qquad \text{(U. 4)}$$

4. ARES (AIR REVITALIZATION SYSTEM)

ARES has the objective to recover oxygen from the CO_2 produced by the crew by physicochemical processes using H_2 as reducer. In a global point of view, the processes that take place are:

- Separate CO_2 from O_2 through an adsorption and desorption process
- Convert CO_2 into H_2O and CH_4 using H_2 as reducer
- Recover the produced H_2O
- Break the H_2O molecule to obtain H_2 and O_2 by an electrolysis process

To achieve each process ARES can be well differentiated in four units that can be composed of determined subsystems (see Table 4-1). Each subsystem is modelled in the same level than MELiSSA subsystems and can be interconnected.

Unit	Subsystem	Symbol
Carbon dioxide Collection Assembly, CCA	Adsorber-Desorber	AD
	Evaporator	E_CCA
	Condenser	C_CCA
	Gas Distributor	GD_CCA
Water Management Unit, WMU	-	WMU
Carbon dioxide Reduction Assembly, CRA	Adiabatic-Isothermal Sabatier Reactor	SR
	Condenser	C_CRA
Oxygen Generator Assembly, OGA	Electrolyser Stack	ES
	Gas Distributor	GD_OGA

Table 4-1: ARES Subsystems

4.1 ARES adaptation for MELiSSA technology

The processes of ARES as an independent technology start with the collection of crew cabin air, which contains the exhaled air from the astronauts (basically nitrogen, oxygen and carbon dioxide), in order to transform CO_2 into water and methane. For the CO_2 reduction the gas must be oxygen free, thus an adsorption unit is necessary.

For a complete LSS, using MELiSSA as a tool base, the carbon dioxide produced in Compartment I can be used. Consequently, the adsorption unit will not be necessary because this CO_2 is exempted from oxygen. Furthermore, Compartment I produces hydrogen that can be used as a reducer in the Sabatier Reactor in case the electrolysis does not produce enough.

Therefore, each subsystem is modelled separately to enable the verification of the optimum configuration.

4.2 The Chemical Compounds from ARES

The chemical compounds that can flow through ARES subsystems are those compounds presented in the MELiSSA gas loop, which are: H_2, O_2, N_2, CO_2, H_2O, NH_3, Acetic acid, Propionic acid, Butyric acid, Valeric acid and Caproic acid. These chemical compounds need to be taken into account in the ARES subsystems to successfully implement ARES into MELiSSA.

4.3 Cooling Water and Cooling Air Circulation

ARES operation requires a flow of cooling water and a flow of cooling air. As shown in Figure 4-1, the cooling water flows firstly through the CCA in order to recover the water vapour. Afterwards, it continues through the CRA where it is used to condense the water in gas phase, which leads to a separation of methane, hydrogen and carbon dioxide. The Sabatier Reactor (CRA) is cooled using a stream of cooling air. There is a heat transfer between the cooling air and the cooling water. The cooling water proceeds to the OGA to exchange heat with the electrolyser's feed water.

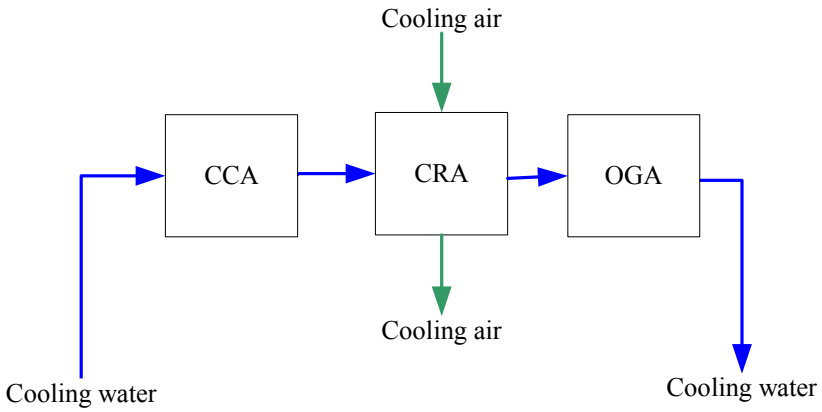


Figure 4-1: Coolants flow

Additionally ARES is composed of several electrical heaters in order to evaporate and/or avoid condensation of water in the gases streams. This subsystem as well as the cooling flow is not represented in the mathematic model.

4.4 CO_2 Collection Assembly (CCA) Mathematic Model Description

The Carbon Dioxide Collection Assembly (CCA) function is to collect the CO_2 from the air through an adsorption process. Furthermore, recuperation systems for condensation water contained in the gas outputs are necessary. Therefore, the CCA is basically composed of the following subsystems:

- Evaporator (E_CCA)
- Adsorber-Desorber (AD)
- Condensers (C_CCA)
- Gas Distributor (GD_CCA)

4.4.1 Evaporator (E_CCA)

4.4.1.1 Description

The CCA evaporator's (E_CCA) function is to produce water vapour, which is utilized at controlled temperature during the CO_2 desorption process. The required thermal energy is supplied by electrical current.

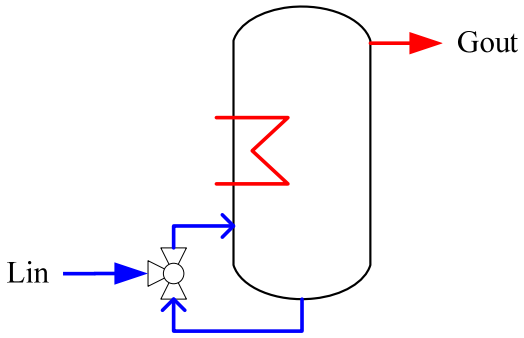


Figure 4-2: Evaporator

Through the mathematic model the evaporation temperature is calculated.

4.4.1.2 Assumption

- All water at the evaporator is evaporated and therefore not accumulated

4.4.1.3 Operational data

Data	Description	Units
Pr	Pressure	Pa

Table 4-2: Operational data for the evaporator

4.4.1.4 Calculation of the temperature

As there is not accumulation, the molar inflow is equal to the molar outflow:

$$Z_{H2O,Lin} = Q_{Lin} \cdot c_{H2O,Lin} = Z_{H2O,Gout} \quad \text{(E. 1)}$$

The temperature can be calculated because it is a function of the water saturation pressure:

$$P_{sat,H2O} = psat\_H2O(TC) \quad \text{(E. 2)}$$

→ With:

psat_H2O(TC) = function within EcosimPro® that returns the value of water saturation pressure for a TC

TC = Temperature in Celsius (ºC)

The volumetric flow can be calculated by using the ideal gas equation:

$$Q_{Gout} = \frac{Z_{H2O,\ Gout} \cdot R \cdot T}{Pr} \quad \text{(E. 3)}$$

The water concentration at the outlet gas is:

$$c_{H2O,Gout} = \frac{Z_{H2O,\ Gout}}{Q_{Gout}} \quad \text{(E. 4)}$$

4.4.2 Adsorber-Desorber

4.4.2.1 Description

The Adsorber-Desorber represents the processes that separate the carbon dioxide from the air. Thus, it can represent several solid amine adsorber beds in which three main operation modes occur: adsorption, desorption and stand-by.

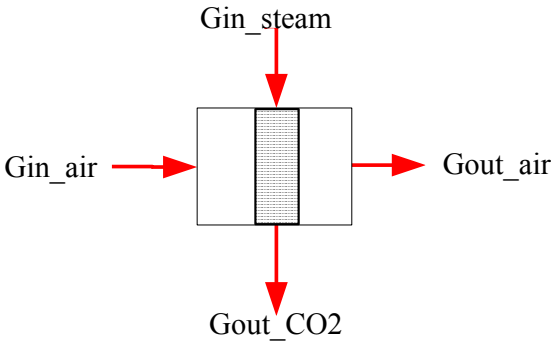


Figure 4-3: Adsorber_Desorber

The objective of the mathematic model is to calculate the volumetric flows and the concentrations at the outlet of the system.

4.4.2.2 Assumptions

- Amine reacts with water to form an amine complex. During adsorption, this complex adsorbs the carbon dioxide from the air, releasing one molecule of water per each carbon dioxide molecule adsorbed. During desorption, the steam flow passes through the solid amine adsorber bed realising the CO_2 and producing again the amine-water complex. The reaction formulae can be summarized as follow:

$$\text{Amine} + H_2O \rightarrow \text{Amine\_}H_2O$$

$$\text{Amine\_}H_2O + CO_2 \rightarrow \text{Amine\_}CO_2 + H_2O \qquad \text{ADSORPTION}$$

$$\text{Amine\_}CO_2 + H_2O \rightarrow \text{Amine\_}H_2O + CO_2 \qquad \text{DESORPTION}$$

- The adsorption only affects the carbon dioxide

4.4.2.3 Operational Data

Adsorber parameters	Description	Units
n_{bed}	Numbers of beds	-
Pr	Pressure	Pa
R	Ideal Gas Constant	J/(K mol)
T	Temperature	K
WS_{Am}	Amine Mass	kg

Table 4-3: Adsorber parameters for the Adsorber-Desorber

Data about adsorption	Description	Units
$H_{CO2,Am}$	Molar fraction of CO2 adsorbed per mol of CO2 that enters and per kg of amine	Kg^{-1}

Table 4-4: Data about adsorption-desorption process

4.4.2.4 *Inflows, Adsorption and Desorption*

The molar flow of each compound at the air inlet is given by equation AD.1, while the molar flow of each compound at the steam inlet is given by equation AD.2:

$$Z_{i,\,in\_air} = Q_{Gin\_air} \cdot c_{i,Gin\_air} \qquad \text{(AD.1)}$$

$$Z_{i,\,in\_steam} = Q_{Gin\_steam} \cdot c_{i,Gin\_steam} \qquad \text{(AD.2)}$$

The molar flow of absorbed carbon dioxide is calculated by using the following equation:

$$Z_{CO2,\,ads} = \left(H_{CO2,\ Am} \cdot WS_{Am} \cdot n_{bed}\right) \cdot Z_{CO2,\,in\_air} \qquad \text{(AD.3)}$$

→ This is also the molar flow of desorption of carbon dioxide

It is assumed that for each carbon dioxide molecule adsorbed one water molecule is released:

$$Z_{H2O,\,free} = Z_{CO2,\,ads} \qquad \text{(AD.4)}$$

4.4.2.5 *Outflows*

In the AD are two outlet streams: air (with fewer CO_2 and more moisture) and the desorbed carbon dioxide.

Air outlet stream ($G_{out\ air}$)

The air at the outlet of the AD system contains less carbon dioxide then at the inlet. The molar outflow of each compound of this stream is the same that the molar inflow, except for the molar flow of water and CO_2:

$$Z_{i,\,Gout\_air} = Z_{i,\,in\_air} \qquad \text{(AD.5)}$$

→ For each compound "i" except H2O and CO2

For H2O and for CO2 the molar outflow at the air outlet is calculated by equation AD.6 and AD.7 respectively.

$$Z_{H2O,\,Gout\_air} = Z_{H2O,\,in\_air} + Z_{H2O,\,free} \qquad \text{(AD.6)}$$

$$Z_{CO2,\,Gout\_air} = Z_{CO2,\,in\_air} - Z_{CO2,\,ads} \qquad \text{(AD.7)}$$

The volumetric outflow is calculated using the ideal gas equation:

$$Q_{Gout\_air} = \frac{\sum_i Z_{i,\ Gout\_air} \cdot R \cdot T}{Pr} \qquad \text{(AD.8)}$$

The concentration of the outlet air is:

$$c_{i,\,Gout\_air} = \frac{Z_{i,\ Gout\_air}}{Q_{Gout\_air}} \qquad \text{(AD.9)}$$

→ For each compound "i"

CO_2 outlet stream, ($G_{out\ CO2}$)

This stream contains the adsorbed carbon dioxide and the excess water vapour that has been used for desorption. The molar outflows of carbon dioxide and of water are respectively:

$$Z_{CO2,\,Gout\_CO2} = Z_{CO2,\,ads} \qquad \text{(AD.10)}$$

$$Z_{H2O,\,Gout\_CO2} = Z_{H2O,\,in\_steam} - Z_{H2O,\,free} \qquad \text{(AD.11)}$$

As previously the volumetric outflow is calculated through the ideal gas equation:

$$Q_{Gout\_CO2} = \frac{\sum_i Z_{i,\,Gout\_CO2} \cdot R \cdot T}{Pr} \qquad \text{(AD.12)}$$

The concentration at the outlet stream of CO_2 is:

$$c_{i,\,Gout\_CO2} = \frac{Z_{i,\,Gout\_CO2}}{Q_{Gout\_CO2}} \qquad \text{(AD.13)}$$

→ For each compound "i"

4.4.3 Gas distributor (GD_CCA)

This subsystem represents a valve with the function to distribute the carbon dioxide coming from the adsorber-desorber. Thus, the quantity of CO_2 that the GD_CCA sends to the SR is controlled. The mathematic model is explained in section 3.8.6.

4.5 CO_2 Reduction Assembly (CRA) Mathematic Model Description

The Carbon Dioxide Reduction Assembly (CRA) function is to reduce the carbon dioxide into methane and water. Thus, this assembly receives a clear gas stream of CO_2 and a gas stream of H_2 in order to produce two outlet streams, one gas of methane and other liquid of water. To achieve this objective, the CRA is basically composed of the following subsystems:

- Sabatier Reactor
- Condenser (C_CRA)

4.5.1 Sabatier Reactor (SR)

4.5.1.1 Description

The Sabatier Reactor is used to convert carbon dioxide and hydrogen to methane and water vapour. The stoichiometric relationship describing Sabatier CO_2 reduction process is given by:

$$CO_2 + 4\,H_2 \Leftrightarrow CH_4 + 2\,H_2O$$

This reaction is exothermic and occurs in presence of a catalyst (ruthenium on aluminium). The process takes place in two consecutive stages; the first under adiabatic conditions and the second under isothermal conditions. Therefore, the first stage takes place in an adiabatic cylindrical reactor tube, while the second one is in an air-cooled reactor.

The system model represents the two Sabatier reactors connected in series. For the calculations the temperature is based on the second reactors', because at this temperature the thermodynamic equilibrium has been reached.

The system is composed of two inputs and one output (see Figure 4-4). The inputs are gas streams of hydrogen and carbon dioxide respectively, and the output is water vapour, methane and the rest of the reactant (either CO_2 or H_2).

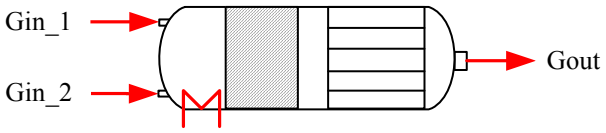


Figure 4-4: Sabatier Reactor

The mathematic model objective is to obtain the volumetric flow and the concentrations of each compound at the reactor outlet.

4.5.1.2 Assumptions

- The reactors work in steady state, thus there is no storage and consequently the accumulation term is zero.
- All the oxygen contained at the inlet stream reacts with hydrogen to produce water.
- The reaction reaches the equilibrium and the "degree of reaction" or equilibrium conversion of H_2 is a function of the pressure and temperature.
- The relation between the hydrogen molar inflow and the carbon molar inflow is more or less the same than the stoichiometric relation.
- The degree of reaction is zero for temperature below 150ºC (423K), because at those temperatures the reaction rate is very slow.

4.5.1.3 Operational Data

Reactor Parameters	Description	Units
Pr	Pressure	Pa
T	Bioreactor Temperature	K
R	Ideal Gas Constant	J/(K mol)

Table 4-5: Operational data for the Sabatier Reactor

4.5.1.4 Stoichiometry

The oxygen present in the inlet stream is eliminated in an initial process within the adiabatic Sabatier reactor through a very fast and highly exothermic reaction (Process 26). The chemical reaction that occurs is as follows:

$$0.5\,O_2 + H_2 \rightarrow H_2O$$

Therefore, the stoichiometric coefficients are fixed as Table 4-6 shows.

Compounds, i	Stoichiometric coefficient, $Y_{i,26}$	Sub index (composition)	
		H	O
O2	-0.5	0	2
H2	-1	2	0
H2O	1	2	1

Table 4-6: Stoichiometry and composition of the O2 reduction process (process 26)

The second process occurring in the reactor is an oxidation-reduction reaction where the carbon dioxide is reduced into methane and the hydrogen is oxidized into water (Process 27). The stoichiometric coefficients for the carbon dioxide reduction are shown in Table 4-7.

Compounds, i	Stoichiometric coefficient, $Y_{i,27}$	Sub index (composition)		
		C	H	O
CH4	1	1	4	0
CO2	-1	1	0	2
H2	-4	0	2	0
H2O	2	0	2	1

Table 4-7: Stoichiometry and composition of the CO2 reduction process (process 27)

4.5.1.5 Balance and Equilibrium Constants

The molar flow of the inlet is calculated through the concentration and volumetric flow at the inlet:

$$Z_{i,in} = Q_{Gin\_1} \cdot c_{i,Gin\_1} + Q_{Gin\_2} \cdot c_{i,Gin\_2} \qquad \text{(SR. 1)}$$

→ The equation accounts for each compound "i", with:

c_{i,Gin_1} = concentration at the gas inlet stream 1 (mol/m^3)

c_{i,Gin_2} = concentration at the gas inlet stream 2 (mol/m^3)

Q_{Gin_1} = volumetric flow of the gas inlet stream 1 (m^3/s)

Q_{Gin_2} = volumetric flow of the gas inlet stream 2 (m^3/s)

$Z_{i,in}$ = molar flow of the inlet (mol/s)

Assuming that the complete oxygen in process 26 is converted, the generation term of this reaction and for each compound can be related to the oxygen molar inflow through the stoichiometric coefficients:

$$G_{i,26} = -Z_{O2,in} \cdot \frac{Y_i}{Y_{O2}} \qquad \text{(SR. 2)}$$

→ For each compound "i". The stoichiometric coefficient of the compounds "i" not shown in Table 4-6 is zero.

It is assumed for process 27 that the limiting chemical reactant is hydrogen. Therefore the generation of this reaction and for each compound depends on the hydrogen "degree of reaction", X_{H2}:

$$G_{i,27} = -X_{H2} \cdot (Z_{H2,in} + G_{H2,26}) \cdot \frac{Y_i}{Y_{H2}} \qquad \text{(SR. 3)}$$

→ for each compound "i". The value of the stoichiometric coefficient, Yi, is zero for the compounds that are not represented in Table 4-7.

It has to be noted that the generation is negative for reactants while it is positive for products.

The outlet molar flow of each chemical compound is calculated by adding the generation terms to its inlet molar flow:

$$Z_{i,out} = Z_{i,in} + G_{i,26} + G_{i,27} \qquad \text{(SR. 4)}$$

→ for each compound "i"

The total molar outflow of the reactor is:

$$Z_{total,out} = \sum_i Z_{i,out} \qquad \text{(SR. 5)}$$

The outlet molar fractions are obtained by dividing the corresponding molar flow through the total molar flow:

$$h_{i,out} = \frac{Z_{i,out}}{Z_{total,out}} \qquad \text{(SR. 6)}$$

The Sabatier reactor's volume is big enough to insure that the reaction reaches equilibrium. The molar equilibrium constant can be expressed for the Sabatier reactor as:

$$Kh = \frac{\prod_{i}^{prod} (h_{i,Gout})^{|Y_i|}}{\prod_{i}^{react} (h_{i,Gout})^{|Y_i|}} = \frac{[h_{CH4,Gout}] \cdot [h_{H2O,Gout}]^2}{[h_{CO2,Gout}] \cdot [h_{H2,Gout}]^4} \qquad \text{(SR. 7)}$$

The pressure equilibrium constant is calculated as a function of reaction temperature according to ([R38] and [R39]):

$$Kp = \exp\left(\frac{28183.19}{T^2} + \frac{17429.79}{T} - 8.2536 \cdot \ln T + 2.8032 \cdot 10^{-3} \cdot T + 33.165\right) \qquad \text{(SR. 8)}$$

→ Kp is in atm^{-2}

→ This equation is only relevant for temperature below 423K

The molar equilibrium constant may be obtained as function of the pressure equilibrium constant according to expression ([R40]):

$$Kh = Kp \cdot \left(\frac{Pr}{1.01325 \cdot 10^5}\right)^2 \qquad \text{(SR. 9)}$$

4.5.1.6 Outputs

Assuming the gas being an ideal gas, the volumetric flow at the outlet can be determined:

$$Q_{Gout} = \frac{Z_{total,out} \cdot R \cdot T}{Pr} \qquad \text{(SR.10)}$$

And the concentration for each compound at the gas outlet is:

$$c_{i,Gout} = \frac{Z_{i,out}}{Q_{Gout}} \qquad \text{(SR.11)}$$

4.5.2 Condenser (C_CRA)

The Condenser of CRA (C_CRA) has the function to recover the water from the gas stream of the Sabatier Rreactor outlet.

It is assumed that the temperature for the condensation is adjusted to result in condensation of only water.

The mathematic model for a condenser is already explained in section 3.8.8.Through these equations the concentration of each compound in the resulting gas, the volumetric outflow and the quantity of condensed water can be obtained.

4.6 Oxygen Generation Assembly (OGA) Mathematic Model

The Oxygen Generation Assembly's (OGA) function is to produce oxygen from water through an electrolysis process. This process takes place in the Electrolyser Stack (ES).

4.6.1 Electrolyser Stack (ES)

4.6.1.1 Description

In chemistry and manufacturing, electrolysis is a method of separating chemically bonded elements and compounds by passing an electric current through them.

Thus, water enters to the electrolyser (ES) (see Figure 4-5) and is oxidized into oxygen that will appear at the anode (the positively charged electrode) and reduced into hydrogen that will appear at the cathode (the negatively charged electrode, where electrons are pumped into the water).

It is very important to take into account that electrolysis of pure water is very slow and, therefore, the use of an electrolyte is required since this substance enables the water to carry an electrical current and complete an electrical circuit. The use of a fixed alkaline electrolyser (KOH concretely) is applied for ARES electrolyser. In this type of electrolysis the electrolyte is fixed in a diaphragm between the anode and cathode (Cat and An in Figure 4-5). Water is evaporated into the diaphragm via a semi-permeable membrane and, therefore, is mixed with the electrolyte. The porous electrodes are attached on both sides of the electrolyte matrix generating hydrogen and oxygen.

Thus, the adjacent gas compartments are free of electrolyte and only filled with the produced wet gases.

Additionally the excess heat has to be removed from the cells. This is performed via a coolant loop, which is simultaneously the feed water loop.

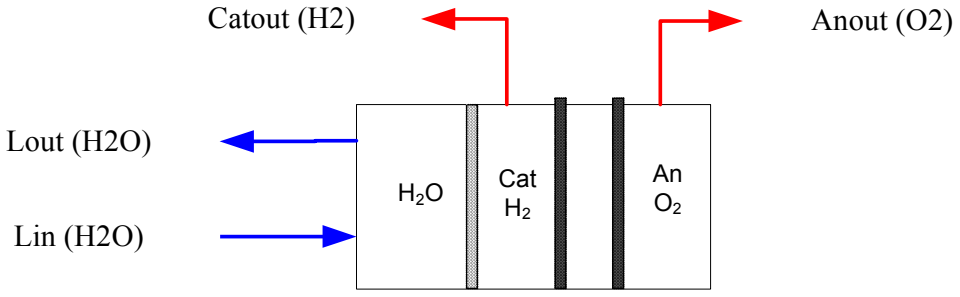


Figure 4-5: Electrolyser Cell

The electrolyser can be composed of several cells connected in series.

4.6.1.2 Assumptions

- The system work in static state, therefore, there is not accumulation
- All gasses behave as an ideal gas

4.6.1.3 Operational Data

Data	Description	Units
A_{cell}	Area of 1 cell	m^2
ef	Current or Faraday efficiency	-
F	Faraday's constant	Coulomb/mol
$f_{KOH,cell}$	Mass fraction of electrolyte per cell	-
$h_{O2,Catdry}$	Molar fraction of oxygen in the dry cathode gas	-
I	Current or electrical electricity	A
k_A	Coefficient to calculate the voltage	$V/(A/m^2)$
k_B	Coefficient to calculate the voltage	$V/(A^2/m^4)$
k_C	Coefficient to calculate the voltage	$V/(A^3/m^6)$
k_D	Coefficient to calculate the voltage	$V/(A^4/m^8)$
k_T	Coefficient to calculate the voltage	V/ºC
n_{cell}	Number of cells	-
Pr_{An}	Gas Anode pressure	Pa
Pr_{Cat}	Gas Cathode pressure	Pa
R	Ideal gas constant	J/(K mol)
RH_{Cat}	Relative humidity in the gas cathode outlet	-
RH_{An}	Relative humidity in the gas anode outlet	-
T	Temperature in the electrolyser	K
T_{ref}	Reference temperature in the voltage calculation	K
Ze	Number of electrons reacting for one molecule of H_2	mol

Table 4-8: Operational data for an electrolyser cell

4.6.1.4 Electrical Equations

The generation of hydrogen and oxygen depend on the quantity of current that flow but also depend on the applied voltage.

The current density, I_D, is defined by:

$$I_D = \frac{I}{A_{cell}} \quad \text{(ES.1)}$$

The electrical performance, that is the fuel cell voltage, is calculated by means of empirical correlation, as follows:

$$U_{cell} = 1.362127 + k_A \frac{I_D}{1000} - k_B \cdot \left(\frac{I_D}{1000}\right)^2 + k_c \left(\frac{I_D}{1000}\right)^3 - k_D \left(\frac{I_D}{1000}\right)^4 - k_T \cdot (T - T_{ref}) \quad \text{(ES. 2)}$$

→ This equation is valid for temperatures between 60 - 95 ºC and for current densities between 500-4000 A/m^2

The reaction of oxidation-reduction takes place if this voltage is about 1.5 – 1.7 V

Because the cells of the stack are electrically connected in series the stack voltage can be calculated using the following equation:

$$U_{stack} = n_{cell} \cdot U_{cell} \quad \text{(ES.3)}$$

The electrical power is the voltage times the current:

$$P_{el} = I \cdot U_{stack} \quad \text{(ES.4)}$$

4.6.1.5 Generation Term

The global reaction that takes place is, in fact, the sum of the semi-reactions that occur in both cathode and anode:

$$2\,H_2O + 2\,e^- \rightarrow H_2 + 2\,OH^- \quad \text{CATHODE REACTION}$$

$$2\,H_2O \rightarrow O_2 + 4\,H^+ + 4\,e^- \quad \text{ANODE REACTION}$$

$$2\,H_2O \rightarrow 2\,H_2 + O_2 \quad \text{GLOBAL REACTION}$$

Knowing the current, the generation term for hydrogen can be calculated through the Faraday law:

$$G_{H2,EL} = ef_F \cdot \frac{I \cdot n_{cell}}{Ze \cdot F} \qquad \text{(ES.5)}$$

Using the stoichiometry of the global reaction, the generation for oxygen and water can be calculated (equations ES.6 and ES.7 respectively):

$$G_{O2,EL} = G_{H2,EL} \cdot \frac{1}{2} \qquad \text{(ES.6)}$$

$$G_{H2O,EL} = G_{H2,EL} \cdot \frac{-1}{1} \qquad \text{(ES.7)}$$

4.6.1.6 Hydraulic Equations and Outputs

The humidity ratio in the gas cathode outlet and gas anode outlet are calculated as follows:

$$H_{H2O,H2\_Cat} = \frac{P_{sat,H2O} \cdot RH_{Cat}}{Pr_{Cat} - P_{sat,H2O} \cdot RH_{Cat}} \qquad \text{(ES.8)}$$

$$H_{H2O,O2\_An} = \frac{P_{sat,H2O} \cdot RH_{An}}{Pr_{An} - P_{sat,H2O} \cdot RH_{An}} \qquad \text{(ES.9)}$$

→ With $P_{sat,H2O}$ being the saturation pressure of water and a function of temperature. It can be calculated through a function that is implemented in EcosimPro® ECCLS library.

→ $P_{sat,H2O\_KOH}$ is the saturation pressure of water in the electrolyte solution and a function of temperature and of KOH concentration. It can be calculated through a function that is implemented in EcosimPro® ECCLS library.

As explained, each cell can be separated in water feed compartment, cathode compartment and anode compartment. Therefore, the balance can be done separately.

Cathode gas outlet

The hydrogen production occurs in the cathode. The molar outflow for hydrogen, oxygen and water in the cathode is:

$$Z_{H2,Catout} = G_{H2,EL} \qquad \text{(ES.10)}$$

$$Z_{O2,Catout} = G_{H2,EL} \cdot \frac{h_{O2,Catdry}}{1 - h_{O2,Catdry}} \quad \text{(ES.11)}$$

$$Z_{H2O,Catout} = G_{H2,EL} \cdot H_{H2O,H2\_Cat} \quad \text{(ES.12)}$$

By knowing the molar outflows of each compound the volumetric outflow of the cathode can be calculated using the ideal gas equation:

$$Q_{Catout} = \frac{Z_{Catout} \cdot R \cdot T}{Pr_{Cat}} \quad \text{(ES.13)}$$

→ with Z_{Catout} being the total molar outflow of the cathode (the sum of each molar outflow of each compound)

The concentration of each compound is given by:

$$c_{i,Catout} = \frac{Z_{i,Catout}}{Q_{Catout}} \quad \text{(ES.14)}$$

→ For each compound that participates in the electrolysis reaction (H2, O2 and H2O)

Anode gas outlet

The oxygen production occurs in the anode. The molar outflow for hydrogen, oxygen and water in the compartment is:

$$Z_{H2,Anout} = 0 \quad \text{(ES.15)}$$

$$Z_{O2,Anout} = G_{O2,EL} - Z_{O2,Catout} \quad \text{(ES.16)}$$

$$Z_{H2O,Anout} = Z_{O2,Anout} \cdot H_{H2O,O2\_An} \quad \text{(ES.17)}$$

As for cathode the volumetric outflow of the anode can be calculated using the ideal gas equation:

$$Q_{Anout} = \frac{Z_{Anout} \cdot R \cdot T}{Pr_{An}} \quad \text{(ES.18)}$$

→ With Z_{Anout} being the total molar outflow of the anode (the sum of each molar outflow of each compound)

The concentration of each compound is given by:

$$c_{i,Anout} = \frac{Z_{i,Anout}}{Q_{Anout}} \quad \text{(ES.19)}$$

→ For each compound that participates in the electrolysis reaction (H2, O2 and H2O)

Water feed compartment

Water entering the compartment is separated from the electrodes by a membrane. Fractions of the water evaporate through the membrane to the electrodes where the electrolysis occurs. The remaining water is uncontaminated with hydrogen, oxygen and electrolyte and is drained off the electrolysis unit. Its molar flow is:

$$Z_{H2O,Lout} = Z_{H2O,Lin} + G_{H2O} - Z_{H2O,Catout} - Z_{H2O,Anout} \quad \text{(ES.20)}$$

→ with $Z_{H2O,Lin}$ being the molar inflow of water

The volumetric outflow is given by:

$$Q_{Lout} = \frac{Z_{H2O,Lout} \cdot M_{H2O}}{1000} \qquad \text{(ES.21)}$$

→ with M_{H2O} being the molecular weight of water

This quantity of water is used for cooling the gasses that leaves the electrolyser.

4.6.2 Gas distributor (GD_OGA)

This subsystem represents a valve with the function to distribute the hydrogen produced in the electrolyser. Thus, the quantity of H_2 that the GD_OGA sends to the SR is controlled. The mathematic model is explained in section 3.8.6.

4.6.3 Water Management Unit (WMU) of ARES Mathematic Model Description

4.6.3.1 Description

This unit represents the processes of water collection and distribution in the ARES unit. The recovered water from the CCA and CRA is part of the feed of the electrolyser and part of the steam needed in the adsorber. Depending on the oxygen production and the quantity of carbon dioxide separated, additional water will be required (Lin_sup in Figure 4-6).

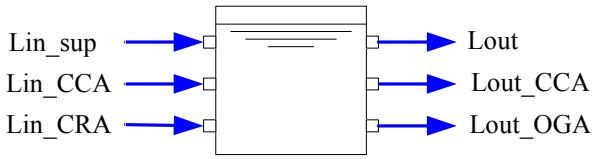


Figure 4-6: Water Management Unit of ARES

The mathematic model is designed to obtain the additional water necessary to fulfil the requirements specified.

4.6.3.2 Operational Data

Data	Description	Units
$Q_{H2O, CCA}$	Volumetric flow of water necessary for the CCA	m^3/s
$Q_{H2O, OGA}$	Volumetric flow of water necessary for the OGA	m^3/s

Table 4-9: Operational data for the Water Management Unit

Recovered Water, Required Water and Additional Water

The recovered water is the sum of the recovered water from the CCA and from the CRA:

$$Q_{H2O,rec} = Q_{H2O,Lin\_CCA} + Q_{H2O,Lin\_CRA} \qquad \text{(WMU.1)}$$

The required flow is the sum of the necessary water for the CCA and for the OGA:

$$Q_{H2O,req} = Q_{H2O,CCA} + Q_{H2O,OGA} \qquad \text{(WMU.2)}$$

Therefore, the additional water is:

$$Q_{H2O,ad} = Q_{H2O,req} - Q_{H2O,rec} \qquad \text{(WMU.3)}$$

4.6.3.3 Outlets

The water of this subsystem is distributed towards the OGA and the CCA whose volumes per time unit are given by the operational data.

The volumetric flow not used to fulfil the requirements is:

$$Q_{Lout} = Q_{Lin\_sup} - Q_{H2O,ad} \qquad \text{(WMU.4)}$$

5. UTU (URINE TREATMENT UNIT)

The UTU objective is to treat the urine produced by the crew using a nitrification process to degrade urea into ammonia and to transform ammonia into nitrates. Thus, the liquid outlet can be used to recover the water and/or can be used to feed the vegetable of MELiSSA.

5.1 The Chemical Compounds from UTU - Urine Composition

The chemical compounds that flow through the UTU are the same compounds presented in the MELiSSA loop. Urine is the main substance of this unit having a variable composition depending on the individual person and the diet. Urine is a liquid and has an ammonia-like odour due to the nitrogenous wastes that represent about 5% of the fluid; the remaining 95% is water. The main constituent of the nitrogenous wastes is urea, a product of protein decomposition.

In addition to the inorganic salts found in the urine, extra concentrations of salts like Na^+, K^+, Ca^+, Mg^{2+}, Cl^-, PO_4^{3-}, and SO_4^{2-} could be present in the urine in a bounded form; bounded to organic matter, proteins, etc. rather than dissolved as such in the urine solution. These bounded forms may be present in higher concentrations. Urine contains also other substances like hormones, specific of the individuals or of the sex as well as heavy metals, which can be harmful.

In accordance to the mathematic model of MELiSSA, the salts and hormones as well as the heavy metals have not been taken into account in the UTU mathematic model, because it is assumed that they are inert and do not accumulate in any subsystem. For further studies they have to be taken into account.

5.2 UTU Mathematic Model Description

UTU is basically composed of three subsystems as shown in Table 5-1.

Set	Subsystem	Symbol
Urine Treatment Unit (UTU)	Dissolver	D_UTU
	Nitrifying Bioreactor	BR_UTU
	Solid-Liquid Separator	SLS_UTU

Table 5-1: UTU subsystems

5.2.1 Dissolver (D_UTU)

5.2.1.1 Description

This subsystem represents a Dissolver (Figure 5-1) which has to dilute the crew's urine. The nitrification process presents some restrictions in relation to the salts load. It is therefore important to dilute the urine (main source of salts) with water at the UTU's input. This dilution is also important for the nitrification process as it decreases the electro conductivity at the entry of the UTU system avoiding a decrease in the nitrification efficiency.

The mathematic model leads to the concentrations of the urine compounds at the outlet of the subsystem (after being diluted).

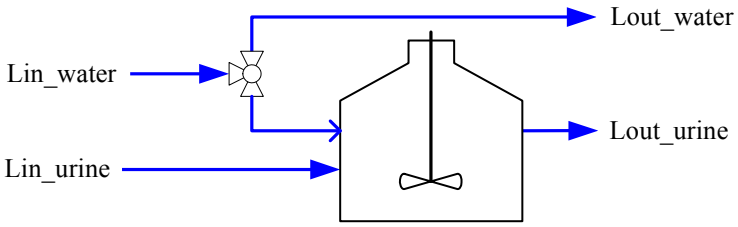


Figure 5-1: Dissolver

5.2.1.2 Operational Data

Data	Description	Units
$R_{H2O,\ urine}$	Cubic meter of water per cubic meter of urine required to dilute urine at the desired conditions	-

Table 5-2: Operational data for the Dissolver

5.2.1.3 Water Requirements

The volumetric flow of additional water to fulfil the dilution conditions is calculated by using the following equation:

$$Q_{H2O,ad} = Q_{Lin\_urine} \cdot R_{H2O,urine} \quad \text{(D.1)}$$

The molar flow of this additional water is:

$$Z_{H2O,ad} = Q_{H2O,ad} \cdot c_{H2O,Lin\_water} \quad \text{(D.2)}$$

Outlets

Urine outlet stream (Lout_urine)

This stream contains the diluted urine.

The molar inflow at the urine inlet for each compound is:

$$Z_{i,Lin\_urine} = Q_{Lin\_urine} \cdot c_{in,Lin\_urine} \quad \text{(D.3)}$$

The volumetric flow is the addition of the volumetric inflow of urine and the volumetric flow of additional water:

$$Q_{Lout\_urine} = Q_{Lin\_urine} + Q_{H2O,ad} \quad \text{(D.4)}$$

The concentration of water in this stream is:

$$c_{H2O,Lout\_urine} = \frac{Z_{H2O,Lin\_urine} + Z_{H2O,ad}}{Q_{Lout\_urine}} \quad \text{(D.5)}$$

The concentration of the remaining compounds is:

$$c_{i,Lout\_urine} = \frac{Z_{i,Lin\_urine}}{Q_{Lout\_urine}} \quad \text{(D.6)}$$

→ for each compound “i” except H2O

Water outlet stream (Lout_water)

This stream contains water not used to dilute. The volumetric flow is the volumetric inflow of water minus the volumetric flow of additional water used to achieve the dilution conditions:

$$Q_{Lout\_water} = Q_{Lin\_water} - Q_{H2O,ad} \quad \text{(D.7)}$$

The concentration of water remains constant, being thus the concentration the same than the inlet concentration.

5.2.2 Nitrifying Bioreactor (BR_UTU)

5.2.2.1 Description

This subsystem represents a nitrifying bioreactor and its function is to transform urea into nitrate.

The nitrification that takes place in this bioreactor is carried out by the same bacteria than colonize the nitrifying bioreactor of Compartment III of MELiSSA: the *Nitrobacter* and the *Nitrosomonas*. The process is similar and the same bioreactor can be used to treat the urine and the liquid coming from Compartment II of MELiSSA. In Figure 5-2 the two kinds of liquid inlets (Lin_urine for urine and Lin for the stream coming from CII) are shown.

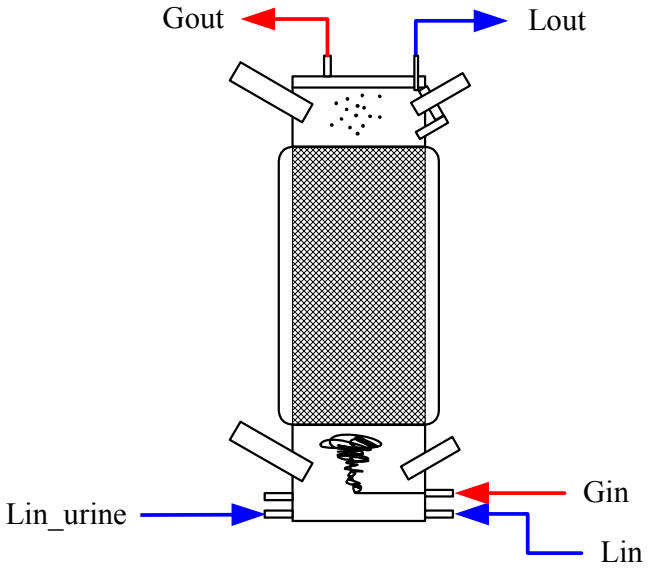


Figure 5-2: Nitrifying Bioreactor

Thus, the formulation used for the UTU bioreactor is the same explained in Compartment III bioreactor, but additionally new equations and new data must be added.

5.2.2.2 Assumptions

- The same as BR_CIII (Section)

Additionally:

- The urine compounds taken into account in the equations are: H_2O, urea, uric acid, creatinine, sulphates (expressed in the form of H_2SO_4) and phosphates (expressed in the form of H_3PO_4).
- Creatinine is not degraded
- There are not accumulation of the salts, hormones and heavy metals contained in urine. These compounds are neglected but under the assumption that they are inert completely and they need to be evacuated or deleted through some concrete process when a recirculation is desired in somewhere of the LSS. That will be studied in future projects.

5.2.2.3 Operational Data

The operational data are the same as explained in BR_CIII (section, table). Additionally the following data are added:

Data	Description	Units
X_{urea}	Urea conversion. It is the percentage of urea decomposed	-
X_{uric}	Uric acid conversion. It is the percentage of uric acid decomposed	-

Table 5-3: Operational data for the UTU Bioreactor

5.2.2.4 Stoichiometry and Generation Due to the Urine Degradation

Urine is composed basically of urea which is oxidised into carbon dioxide and ammonia according to the following reaction:

$$CH_4ON_2 + H_2O \rightarrow 2NH_3 + CO_2$$

The generation term of urea through this oxidation process (ox1) is a function of the urea conversion:

$$G_{urea,ox1} = -X_{urea} \cdot Z_{urea,in\_total} \qquad \text{(BR\_UTU.1)}$$

→ With:

$$Z_{urea,total\_in} = Q_{Lin\_urine} \cdot c_{urea,Lin\_urine} + Q_{Lin} \cdot c_{urea,Lin} \qquad \text{(BR\_UTU.2)}$$

Q_{Lin_urine} = Volumetric flow at the liquid urine inlet (m^3/s)

c_{urea,Lin_urine} = Molar concentration of urea at the liquid urine inlet (mol/s)

Q_{Lin} = Volumetric flow at the liquid inlet (m^3/s)

$c_{urea,Lin}$ = Molar concentration of urea at the liquid inlet (mol/s)

The generation of the remaining compounds for this process can be determined through stoichiometry:

$$G_{i,ox1} = G_{urea,ox1} \cdot \frac{Y_{i,ox1}}{Y_{urea,ox1}} \qquad \text{(BR\_UTU.3)}$$

→ Equation for the compounds "i" = $H2O$, $CO2$, $NH3$, and with:

$$Y_{urea,ox1} = -1$$

$$Y_{H2O,ox1} = -1$$

$$Y_{CO2,ox1} = +1$$

$$Y_{NH3,ox1} = +2$$

→ For the remaining compounds the generation term in this oxidation is zero:

$$G_{i,ox1} = 0$$

The other oxidized urine compound is the uric acid. The products of this process are also carbon dioxide and ammonia:

$$C_5H_4O_3N_4 + 4\,H_2O + 0.5\,O_2 \rightarrow 5\ CO_2 + 4\,NH_3$$

As in the previous case, the uric generation term for this oxidation (ox2) is a function of uric conversion and the steps to obtain the generation of each compound, $G_{i,ox2}$, follow the same way.

Therefore, the global generation term of each compound in the UTU bioreactor (see equation BR_UTU.4) takes into account the two oxidation processes that the urine compounds undergo, urea oxidation and uric oxidation ($G_{i,ox1}$ and $G_{i,ox2}$ respectively), and the generation term due to the two oxidation processes that compose the nitrification (G_{i,BR_CIII}). The latter is obtained as is explained in section 3.6.4

$$G_{i,BR\_UTU} = G_{i,BR\_CIII} + G_{i,ox1} + G_{i,ox2} \qquad \text{(BR\_UTU.4)}$$

→ For each compound “i”

5.2.3 Solid_Liquid Separator (SLS_UTU)

As UTU is composed of one bioreactor, there is biomass production and consequently a Solid Liquid Separator is required. The representation of this subsystem is explained in section 2.2.8.4.

6. WTU (WATER TREATMENT UNIT)

The WTU objective is to recover hygiene and potable water from the crew (showers), from the condensate coming from the HPC of MELiSSA and from the liquid output of the UTU. The hygiene water recovered will be used for crew hygiene and for others uses (as a dissolvent in BPU of MELiSSA, as a feed in the ES of ARES, etc).

6.1 WTU Chemical Compounds

The water that the WTU receives is composed of inorganic salts, salts of Na^+, K^+, Ca^+, Mg^{2+}, Cl^-, PO_4^{3-}, and SO_4^{2-}, heavy metals like Ni, Ag, Zn and Cu, and organic matter. Through the processes in the WTU, the concentration of these compounds will be reduced considerably although the concentration of these compounds is not specified.

6.2 WTU Mathematic Model Description

The WTU is basically composed of two subsystems (see table)

Set	Subsystem	Symbol
Water Treatment Unit (UTU)	Grey Water Treatment Unit	GWTU
	Water Potabiliser	WP

Table 6-1: WTU subsystems

6.2.1 Grey Water Treatment Unit (GWTU)

6.2.1.1 Description

The GWTU model represents three successive membrane units: one nanofiltration unit based on mineral membranes, and two reverse osmosis units. The role of the set of membranes is to eliminate turbidity and to eliminate organic molecules as well as ionic compounds (salts) from the water coming from the crew chamber, from the condensate and from other subsystems, like UTU (see Figure 6-1).

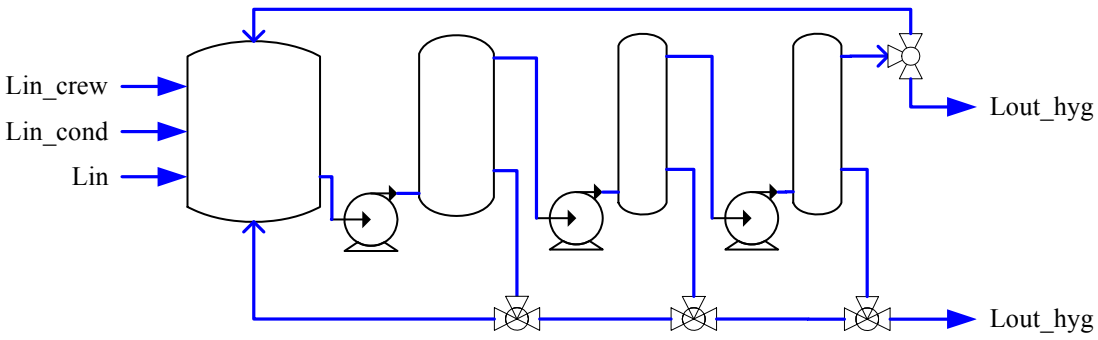


Figure 6-1: Grey Water Treatment Unit

The mathematic model applied to this unit consists of calculating the recovered hygiene water.

6.2.1.2 Operational Data

Data	Description	Units
R_{water}	Percentage of recovery from the total water inflow	-

Table 6-2: Operational data for the GWTU

6.2.1.3 Outlets

The water from the crew, the condensate and the waste water coming from others subsystems are joined in one stream and undergo processes of decontamination that are not able to recover 100% of the water to hygiene level standard. Therefore, there are two outputs: hygiene water and waste water.

The recovery percentage given as a data must be coherent with the osmotic pressure. It has to be a value that does not lead to an excessive osmotic pressure. To calculate the osmotic pressure through the Van't Hoff equation it is necessary to know the diluted ion concentration but the mathematical model does not calculate all the concentration of the salts and ions that exists in the system. Therefore, the recovery percentage must be very similar to the experimental values obtained in the technologies of grey water treatment.

The volumetric flow of the inflow water, Q_{Lin_total}, is the sum of the waste water coming from the crew, from the condensation and from others subsystems (like UTU).

The hygiene water obtained is proportional directly to the total inflow:

$$Q_{Lout\_hyg} = R_{water} \cdot Q_{Lin\_total} \qquad \text{(GWTU.1)}$$

The non-recovered water (waste water) is the total inflow minus the recovered water:

$$Q_{Lout\_waste} = Q_{Lin\_total} - Q_{Lout\_hyg} \qquad \text{(GWTU.2)}$$

The concentration of water in both outlet streams is:

$$c_{H2O,Lout\_hyg} = c_{H2O,Lout\_waste} = \frac{Q_{Lin\_crew} \cdot c_{H2O,Lin\_crew} + Q_{Lin\_cond} \cdot c_{H2O,Lin\_cond} + Q_{Lin} \cdot c_{H2O,Lin}}{Q_{Lin\_total}} \qquad \text{(GWTU.3)}$$

6.2.2 Water Potabiliser (WP)

6.2.2.1 Description

The hygiene water obtained through the GWTU is not potable and therefore needs further treatment to reach the level of potable water.

This subsystem represents the obtaining of potable water. Thus certain quantity of the hygiene water is potabilized (see Figure 6-2).

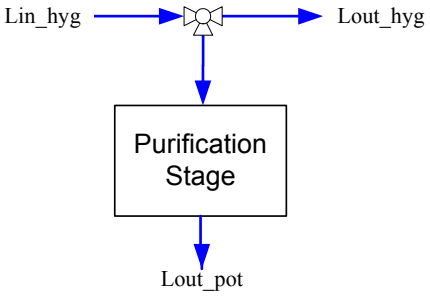


Figure 6-2 Water Potabiliser

The addition of minerals as well as disinfectants, like chlorine, in the purification stage to obtain potable water has not been taken into account in the mathematic model.

6.2.2.2 Operational Data

Data	Description	Units
R_{pot}	Percentage of potable water recovered from the hygiene water	-

Table 6-3: Operational data for the Water Potabiliser

6.2.2.3 Outlets

The potable water obtained is:

$$Q_{Lout\_pot} = R_{pot} \cdot Q_{Lin\_hyg} \quad \text{(WP.1)}$$

The hygiene water not used as potable is:

$$Q_{Lout\_hyg} = Q_{Lin\_hyg} - Q_{Lout\_pot} \quad \text{(WP.2)}$$

It is assumed that the concentration of water remains constant.

7. AIR QUALITY SENSORS

Two air quality sensors are currently under development in Europe, MIDASS and ANITA. These instruments will be central in the determination of the air quality in closed habitats where air is recycled in closed loop using regenerative process. The ANITA sensor is in a well advanced level of maturity and it has been recently launched to the ISS (flight STS 118) for experimental use onboard [R 40].

Although the MIDASS fundamental principles have also been proven, the instrument design is still under development phase.

Both instruments are designed for reduced envelope, mass and power consumption needs (e.g. two standard mid-deck lockers, around 50 kg and around 100 W, respectively).

7.1 MIDASS

MIDASS (Microbial Detection In Air System for Space) is a technology intended to develop an integrated monitoring system for detection and quantification of microbial contamination in air. This technology, and the associated instrument, is justified to detect and prevent microbial contamination risks induced by the air recirculation obtained through the regenerative processes implemented in closed loop LSS envisaged in long duration space manned missions.

7.2 ANITA

ANITA (Analysing Interferometer for Ambient Air) is a permanent continuous trace gas monitoring system that can detect and quantify online and with high time resolution 30 trace gases simultaneously with sub-ppm detection limits in addition to the always in habitat present background gases carbon dioxide and water vapour [R 40]. This air quality monitor allows therefore the detection and monitoring of trace gas dynamics of the spacecraft / habitat atmosphere, providing continuous air monitoring as well as crew warning capability in case of malfunctions.

APPENDIX: ECOSIMPRO® EUROPEAN LSS LIBRARY

A.1 Overview of European Life Support System Technologies Library

A.1.1 Components of the European Life Support System Technologies Library

Component Type Name	Item Description
Adsorber_Desorber	CO_2 Adsorber Bed
Arthrospira_Washing	Staged cleaning of Arthrospira Platensis
Atmosphere_ Generator	Atmosphere Generator
Biomass_Pretreatment_Unit	Biomass collector and shredder
CI_Bioreactor	Bioreactor of Compartment I
CII_Bioreactor	Bioreactor of Compartment II
CIII_Bioreactor	Bioreactor of Compartment III
CIVa_Bioreactor	Bioreactor of Compartment Iva
Condenser	Water Vapor Condenser
Crew_Compartment	Crew Compartment
Dissolver_UTU	Dissolver to dilute urin for urine treatment unit
Electrolyzer_Stack	Electrolyzer Stack
Evaporator	Evaporator
Food_Treatment_Unit	Processor for food ingredients
Gas_Collector	Gas Collector (CDC and MOC)
Gas_Distributor	Stream Divisor for Gas
Grey_Water_Treatment_Unit	Processor for used water. It is the Grey Water Treatment Unit
Higher_Plants_Chamber	Higher Plants Chamber
Liquid_Collector	Collector to merge liquid streams
Liquid_Collector_Distributor	Processor for Liquids
Liquid_Distributor	Stream Divisor for Liquids
Plants Chamber	Description of the crops that belongs to the plant chamber
Purge_Gas	Purge for gas
Purge_Liquid	Purge for liquid
Sabatier_Reactor	Sabatier Reactor (Adiabatic SR and Isothermal SR)
Sold_Distributor	Stream Divisor for Solids
Solid_Liquid_Separator	Separator for isolating solids from liquids
Union_Point_Gas	Union point. It is a system to join gaseous outside streams with gaseous inside streams.
Union_Point_Liquid	Union point. It is a system to join liquid outside streams with liquid inside streams.
Water_Management_ARES	Water Management Unit
Water_Potabilizer	Processing hygene water to potable water

A.1.2 Chemical Compounds that appear in the MELiSSA loop

COMPOUND	SUB-INDEX
Acetic Acid	Ac
Ammoniac	NH3
Biomass of *Arthrospira platensis*	Ap
Biomass of Additional Food	AdF
Biomass of Eatable Part of Plants	HPc
Biomass of Microorganisms in Compartment I	BIO_1
Biomass of *Nitrosomonas europaea* and *Nitrobacter winogradskyi*	New
Biomass of *Rhodospirillum rubrum*	Rr
Butyric Acid	But
Caproic Acid	Cap
Carbohydrates	Ch
Creatinine	creat
Deoxyribonucleic Acid	DNA
Exopolysaccharides	Ex
Faeces	Fc
Hydrogen	H2
Lipids	lip
Methane	CH4
Nitrate	HNO3
Nitrogen	N2
Non-degradable organic matter	ND
Oxygen	O2
Phosphate	H3PO4
Propionic Acid	Prop
Proteins	prot
Residual Biomass	RB
Residual Biomass of Plants	HPre
Residual Organic Matter	Re
Ribonucleic Acid	RNA
Solid Urine	SU
Sulphate	H2SO4
Urea	urea
Ureic acid	uric
Urine	urine
Valeric Acids	Val
Water	H2O

A.1.3 Enumerative Data Types

A.1.3.1 *Enumerative Data Type* `Elements`

It defines the chemical elements that contained in chemical compounds.

```
ENUM Elements = {C,H,O,N,S,P}
```

A.1.3.2 Enumerative Data Type Crops

It defines the crop constituents that participle in the Plant Chamber.

```
ENUM Crops = {tomato,potato,wheat,rice,salad,soybean,onion,spinach}
```

A.1.3.3 Enumerative Data Type Chemicals

It defines the chemical constituents that can participate in the systems

```
ENUM Chemicals=
{Ac,Prop,But,Val,Cap,O2,CO2,NH3,H2,N2,H2O,HNO3,H3PO4,H2SO4,
Rr,New,Fc,HPre,RB,prot,ch,lip,DNA,RNA,Re,BIO_1,CH4,inert,ex,
Ap,HPc,adF,solid_urine,urea,uric,creat}
```

A.1.3.4 Derived Types – SET_OF Dynamic Enumeration Types

It defines a set of chemicals that are used for different groups, which are:

- A set that flow through the system
  ```
  SET_OF (Chemicals)
  Compounds={Ac,Prop,But,Val,Cap,O2,CO2,NH3,H2,N2,H2O,HNO3,
  H3PO4,H2SO4,CH4,urea,uric,creat,Rr,New,Fc,HPre,RB,Ap,HPc}
  ```
- A set of the main biomelecules of the biomass from R. rubrum
  ```
  SET_OF (Chemicals) m_Rr= {prot,ch,lip,DNA,RNA}
  ```
- A set of the main biomelecules of the biomass from A. platensis
  ```
  SET_OF (Chemicals) m_Ap= {prot,ch,lip,DNA,ex}
  ```
- A set of the main biomelecules of the biomass from additional food
  ```
  SET_OF (Chemicals) m_ad= {prot,ch,lip}
  ```
- A set of biomass of the system
  ```
  SET_OF (Chemicals) Biomass = {Rr,New,Fc,HPre,RB,Ap}
  ```
- A set of non-comestible biomass
  ```
  SET_OF (Chemicals) Biomass_NC = {Rr,New,Fc,HPre}
  ```
- A set of comestible biomass
  ```
  SET_OF (Chemicals) Food_components = {HPc,Ap,Fad}
  ```
- A set of volatile fatty acids
  ```
  SET_OF (Chemicals) VFA= {Ac,Prop,But,Val,Cap}
  ```
- A set of acid-base compounds (only those acids or bases that are also in gas phase)
  ```
  SET_OF (Chemicals) Acid_base= {Ac,Prop,But,Val,Cap,CO2,NH3,H2O}
  ```
- A set of non acid-base compounds
  ```
  SET_OF (Chemicals) No_Acid_base=
  {H2,N2,HNO3,H3PO4,H2SO4,Rr,New,Fc,HPre,RB,O2,HPc,Ap,
  CH4,urea,uric,creat}
  ```
- A set of compounds contained in liquid phase only

```
SET_OF (Chemicals) Only_Liquid=
{H3PO4,HNO3,H2SO4,Rr,New,Fc,HPre,RB,HPc,Ap,urea,uric,creat}
```

- A set of bi-phasic compounds
```
SET_OF (Chemicals) Gas_Liquid=
{Ac,CO2,H2,NH3,O2,H2O,But,Cap,Prop,Val,N2,CH4}
```
- A set of urine solid compounds
```
SET_OF (Chemicals) Urine_solid_compounds={urea,uric,creat}
```
- A set of urine compounds
```
SET_OF (Chemicals) Urine_compounds=
{urea,uric,creat,H2O,H2SO4,H3PO4}
```
- A set of water compunds
```
SET_OF (Chemicals) Water = {H2O}
```
- Process 1: RB → prot + ch + lip+ Re
```
SET_OF (Chemicals) Process1 = {prot,ch,lip,RB,Re}
```
- Process 2: Re → ch+ NH_3 + H_2SO_4 + H_3PO_4 + inert
```
SET_OF (Chemicals) Process2 = {ch,NH3,H2SO4,H3PO4,inert,Re}
```
- Process 3: ch+ NH_3 + H_2O → Prop + Ac + CO_2 + BIO_1
```
SET_OF (Chemicals) Process3 = {Ac,Prop,CO2,NH3,H2O,ch,BIO_1}
```
- Process 4: prot+ H_2O → Cap + Val + But + Prop + Ac + H_2 + CO_2 + BIO_1
```
SET_OF (Chemicals) Process4 =
{prot,Ac,Prop,But,Val,Cap,CO2,H2,NH3,H2O,BIO_1}
```
- Process 5: lip + NH_3 + H_2O → Ac + H_2 + BIO_1
```
SET_OF (Chemicals) Process5 = {Ac,H2,NH3,H2O,lip,BIO_1}
```
- Process 6: Prop + NH_3 + H_2O → Ac + H_2 + CO_2 + BIO_1
```
SET_OF (Chemicals) Process6 = {Prop,CO2,Ac,H2,NH3,H2O,BIO_1}
```
- Process 7: But+ NH_3 + H_2O → Ac + H_2 + BIO_1
```
SET_OF (Chemicals) Process7 = {But,Ac,H2,NH3,H2O,BIO_1}
```
- Process 8: Val + NH_3 + H_2O → Ac + H_2 + CO_2 + BIO_1
```
SET_OF (Chemicals) Process8 = {Val,CO2,Ac,H2,NH3,H2O,BIO_1}
```
- Process 9: Cap + NH_3 + H_2O → Ac + H_2 + BIO_1
```
SET_OF (Chemicals) Process9 = {Cap,Ac,H2,NH3,H2O,BIO_1}
```
- Process 10: CO_2+ H_2 + NH_3 → CH_4 + H_2O + BIO_1
```
SET_OF (Chemicals) Process10 = {CO2,H2,NH3,CH4,H2O,BIO_1}
```
- Process 11: Ac + NH_3 → CO_2 + CH_4 + H_2O + BIO_1
```
SET_OF (Chemicals) Process11 = {Ac,NH3,CO2,CH4,H2O,BIO_1}
```
- Process 12: BIO_1 + H_2O → NH_3 + H_2 + CO_2
```
SET_OF (Chemicals) Process12 = {NH3,CO2,H2,H2O,BIO_1}
```
- Process 13: RB + H_2O → ch + prot + lip + H_2SO_4 + H_3PO_4 + Ac + Prop + But + Val + Cap + CO_2 + H_2 + CH_4 + NH_3 + inert + BIO_1, with ch+prot+lip+inert+BIO1 = ND
```
SET_OF (Chemicals) Process13 =
{Ac,Prop,But,Val,Cap,O2,CO2,NH3,H2,H2O,HNO3,H3PO4,H2SO4,RB,prot
,ch,lip,Re,inert,BIO_1,CH4}
```
- Process 14: Ac + NH_3 + H_2SO_4 + H_3PO_4 → Rr + CO_2 + H_2O
```
SET_OF (Chemicals) Process14 = {Ac,NH3,H2SO4,H3PO4,CO2,H2O,Rr}
```
- Process 15: Prop+ NH_3 + H_2SO_4 + H_3PO_4 → Rr + CO_2 + H_2O
```
SET_OF (Chemicals) Process15 =
{Prop,NH3,H2SO4,H3PO4,CO2,H2O,Rr}
```

- Process 16: But + NH_3 + H_2SO_4 + H_3PO_4 → Rr + CO_2 + H_2O
  `SET_OF (Chemicals) Process16 = {But,NH3,H2SO4,H3PO4,CO2,H2O,Rr}`
- Process 17: Val+ NH_3 + H_2SO_4 + H_3PO_4 → Rr + CO_2 + H_2O
  `SET_OF (Chemicals) Process17 = {Val,NH3,H2SO4,H3PO4,CO2,H2O,Rr}`
- Process 18: Cap+ NH_3 + H_2SO_4 + H_3PO_4 → Rr + CO_2 + H_2O
  `SET_OF (Chemicals) Process18 = {Cap,NH3,H2SO4,H3PO4,CO2,H2O,Rr}`
- Process19: CO_2 + NH_3 + H_2SO_4 + H_3PO_4 + O_2 → New + HNO_2 + H_2O
  `SET_OF (Chemicals) Process19 = {CO2,NH3,H2SO4,H3PO4,O2,New,H2O}`
- Process 20: NH_3 + O_2 → HNO_2 + H_2O
  `SET_OF (Chemicals) Process20 = {NH3,O2,H2O}`
- Process 21: CO_2 + NH_3 + HNO_2 + H_2SO_4 + H_3PO_4 + O_2 → New + HNO_3 + H_2O
  `SET_OF (Chemicals) Process21 = {CO2,NH3,H2SO4,H3PO4,HNO3,O2,New,H2O}`
- Process 22: HNO_2 + O_2 → HNO_3
  `SET_OF (Chemicals) Process22 = {HNO3,O2}`
- Process 23: CO_2 + HNO_3 + H_2SO_4 + H_3PO_4 → Ap + O_2 + H_2O
  `SET_OF (Chemicals) Process23 = {CO2,HNO3,H2SO4,H3PO4,O2,H2O,Ap}`
- Process 24: CO_2 + HNO_3 + NH_3 + H_2SO_4 + H_3PO_4 → HPnc + HPc + O_2 + H_2O
  With HPnc + HPc = Crops
  `SET_OF (Chemicals) Process24 = {CO2,HNO3,NH3,H2SO4,H3PO4,O2,H2O}`
- Process 25: FOOD + O_2 → FAECES + (UREA + UREIC + CREATININE) + H_2SO_4 + H_3PO_4 + CO_2 + H_2O
  `SET_OF (Chemicals) Process25 = {CO2,O2,H2O,solid_urine,H2SO4,H3PO4,Fc}`
- Process26: O_2 + H_2 → H_2O
  `SET_OF (Chemicals) Process26 = {O2,H2,H2O}`
- Process 27: CO_2 + H_2 → H_2O + CH_4
  `SET_OF (Chemicals) Process27 = {CO2,H2,H2O,CH4}`
- Process28: H_2O → H_2 + O_2
  `SET_OF (Chemicals) Process28 = {O2,H2,H2O}`
- Process29: CH_4ON_2 + H_2O → CO_2 + NH_3
  `SET_OF (Chemicals) Process29 = {CO2,NH3,urea,H2O}`
- Process30: $C_5H_4O_3N_4$ + H_2O + O_2 → CO_2 + NH_3
  `SET_OF (Chemicals) Process30 = {CO2,NH3,uric,H2O,O2}`

A.1.4 Library Variables

The library defines the following constant variables:

- Molecular weights of single elements (kg/mol) (C, H, O, N, S, P)

```
CONST REAL mol_weight[Elements] = { 0.012011, 0.0010079,
0.0159994, 0.0140067, 0.032066, 0.0309738 }
```

- CHONSP composition of compounds (Ac, Prop, But, Val, Cap, O2, CO2, NH3, H2, N2, H2O, HNO3, H3PO4, H2SO4, CH4, urea, uric, creat, Rr, New, Fc, HPre, RB, Ap, HPc)

```
CONST REAL C_compound[Compounds] = { 2, 3, 4, 5, 6, 0, 1, 0, 0,
0, 0, 0, 0, 0, 1, 1, 5, 4, 0, 0, 0, 0, 0, 0, 0}
CONST REAL H_compound[Compounds] = { 4, 6, 8, 10, 12, 0, 0, 3,
2, 0, 2, 1, 3, 2, 4, 4, 4, 7, 0, 0, 0, 0, 0, 0, 0}
CONST REAL O_compound[Compounds] = { 2, 2, 2, 2, 2, 2, 2, 0, 0,
0, 1, 3, 4, 4, 0, 1, 3, 1, 0, 0, 0, 0, 0, 0, 0}
CONST REAL N_compound[Compounds] = { 0, 0, 0, 0, 0, 0, 0, 1, 0,
2, 0, 1, 0, 0, 0, 2, 4, 3, 0, 0, 0, 0, 0, 0, 0}
CONST REAL S_compound[Compounds] = { 0, 0, 0, 0, 0, 0, 0, 0, 0,
0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
CONST REAL P_compound[Compounds] = { 0, 0, 0, 0, 0, 0, 0,  0,
0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0}
```

- CHONSP composition in process 1 (prot, ch, lip, RB, Re)

```
CONST REAL C_p1[Process1] = { 1, 1, 1, 0, 0}
CONST REAL H_p1[Process1] = { 1.55386, 1.6667, 2, 0, 0 }
CONST REAL O_p1[Process1] = {0.28354, 0.8333, 0.125, 0, 0}
CONST REAL N_p1[Process1] = { 0.2693, 0, 0, 0, 0 }
CONST REAL S_p1[Process1] = { 0, 0, 0, 0, 0 }
CONST REAL P_p1[Process1] = { 0, 0, 0, 0, 0 }
```

- CHONSP composition in process 2 (ch, NH_3, H_2SO_4, H_3PO_4, inert, Re)

```
CONST REAL C_p2[Process2] = { 1, 0, 0, 0, 0, 0 }
CONST REAL H_p2[Process2] = { 1.6667, 3, 2, 3, 0, 0 }
CONST REAL O_p2[Process2] = { 0.8333, 0, 4, 4, 0, 0 }
CONST REAL N_p2[Process2] = { 0, 1, 0, 0, 0, 0 }
CONST REAL S_p2[Process2] = { 0, 0, 1, 0, 0, 0 }
CONST REAL P_p2[Process2] = { 0, 0, 0, 1, 0, 0 }
```

- CHONSP composition in process 12 (NH_3, CO_2, H_2, H_2O, BIO_1)

```
CONST REAL C_p12[Process12] = { 0, 1, 0, 0, 5 }
CONST REAL H_p12[Process12] = { 3, 0, 2, 2, 7 }
CONST REAL O_p12[Process12] = { 0, 2, 0, 1, 2 }
CONST REAL N_p12[Process12] = { 1, 0, 0, 0, 1 }
```

A.1.5 Functions

The functions used are:

Dissociation constant (k_i)

Symbol	Function	Variables	Symbol	Description	Units
Diss_const	T, Compound, pH	$k_{a,i}$	k1	Acidity constant of compound "i"(acid compound)	-
		$k_{a1,i}$	k1	First acidity constant of compound "i"(bi-acid compound)	-
		$k_{a2,i}$	k2	Second acidity constant of compound "i"(bi-acid compound)	-
		$k_{b,i}$	k1	Basicity constant of compound "i" (base compound)	-
		k_w	k1	Ionic product of water	-
		A	A	First Coefficient of Antoine Law (K)	K
		B	B	Second coefficient of Antoine Law	-
		C	C	Third coefficient of Antoine Law (K**-1)	K^{-1}
		D	D	Fourth coefficient of Antoine Law	-

Gas-Liquid equilibrium constant, Alpha (α_i)

Symbol	Function	Variables	Symbol	Description	Units
Alpha	T, Compound	A	A	First coefficient of Antoine Law	K
		B	B	Second coefficient of Antoine Law	K
		C	C	Third coefficient of Antoine Law	K
		D	D	Fourth coefficient of Antoine Law	K
		VM	VM	Molecular volume	L/mol
		no	no	Number of moles of water in one litre	mol/L
		Kp_i	Kp	Partition coefficient	-

Molecular Weight (M_i)

Symbol	Function	Variable	Symbol	Description	Units
MolecularWeight	Compound	M_E	mol_weight[Elements]	Molecular weight of each element	kg/mol

Saturation pressure of water ($P_{sat,H2O}$)

Symbol	Function of
psat_H2O	TC (Temperature in centigrade)

Saturation pressure of water in an electrolyte (KOH) solution ($P_{sat,H2O\_KOH}$)

Symbol	Function of
psat_H2O_KOH	TC (Temperature in centigrade), cm_KOH (KOH mass concentration)

A.2 Port Types

A.2.1 Port Liquid

A.2.1.1 Description

The Liquid Port is defining the liquid connections in the MELiSSA System.

A.2.1.2 Graphics

Connections between ports of this type are represented in the model flow-sheet in solid blue lines.

Liquid

A.2.1.3 Construction Parameters

Within the liquid port is defined a subset of Chemicals

```
SET_OF (Chemicals) mix
```

A.2.1.4 Variables

SYMBOL	TYPE	DESCRIPTION	UNITS
C[Biomass]	EQUAL REAL	Molar carbon amount in dry biomass	-
Con[mix]	EQUAL REAL	Total concentration of each compound	mol/m^3
f_ch[Biomass]	EQUAL REAL	Mass fraction of carbohydrates in dry biomass	-
f_H2O[Biomass]	EQUAL REAL	Mass fraction of water in damp biomass	-
f_lip[Biomass]	EQUAL REAL	Mass fraction of lipids in dry biomass	-
f_prot[Biomass]	EQUAL REAL	Mass fraction of protons in dry biomass	-
H[Biomass]	EQUAL REAL	Molar hydrogen amount in dry biomass	-
M[Biomass]	EQUAL REAL	Molecular Weight of dry biomass	-
N[Biomass]	EQUAL REAL	Molar nitrogen amount in dry biomass	-
O[Biomass]	EQUAL REAL	Molar oxygen amount in dry biomass	-
P[Biomass]	EQUAL REAL	Molar phosphorus amount in dry biomass	-
Q	SUM REAL	Volumetric flow	m^3/s
S[Biomass]	EQUAL REAL	Molar sulphur amount in dry biomass	-

A.2.2

Intentionally left blank

A.2.3 Port `Gas`

A.2.3.1 Description

The Gas Port is defining the gas connections in the MELiSSA System.

A.2.3.2 Graphics

Connections between ports of this type are represented in the model flow-sheet in slid red lines.

Gas

A.2.3.3 Construction Parameters

Within the liquid port is defined a subset of Chemicals

```
SET_OF (Chemicals) mix
```

A.2.3.4 Variables

SYMBOL	TYPE	DESCRIPTION	UNITS
`Con[mix]`	EQUAL REAL	Total concentration of each compound	mol/m^3
`Q`	SUM REAL	Volumetric flow	m^3/s

A.2.4 Port `Solid`

A.2.4.1 Description

The Solid Port is defining the solid connections in the MELiSSA System.

A.2.4.2 Graphics

Connections between ports of this type are represented in the model flow-sheet in solid brown lines.

Solid

A.2.4.3 Construction Parameters

Within the liquid port is defined a subset of Chemicals

```
SET_OF (Chemicals) mix
```

A.2.4.4 Variables

SYMBOL	TYPE	DESCRIPTION	UNITS
C[Biomass]	EQUAL REAL	Molar carbon amount in dry biomass	-
Con[mix]	EQUAL REAL	Total concentration of each compound	mol/m^3
f_ch[Biomass]	EQUAL REAL	Mass fraction of carbohydrates in dry biomass	-
f_H2O[Biomass]	EQUAL REAL	Mass fraction of water in damp biomass	-
f_lip[Biomass]	EQUAL REAL	Mass fraction of lipids in dry biomass	-
f_prot[Biomass]	EQUAL REAL	Mass fraction of proteins in dry biomass	-
H[Biomass]	EQUAL REAL	Molar hydrogen amount in dry biomass	-
M[Biomass]	EQUAL REAL	Molecular Weight of dry biomass	-
N[Biomass]	EQUAL REAL	Molar nitrogen amount in dry biomass	-
O[Biomass]	EQUAL REAL	Molar oxygen amount in dry biomass	-
P[Biomass]	EQUAL REAL	Molar phosphorus amount in dry biomass	-
Q	SUM REAL	Volumetric flow	m^3/s
S[Biomass]	EQUAL REAL	Molar sulphur amount in dry biomass	-

A.2.5 Port `Plants`

A.2.5.1 Description

The Plants Port is defining the higher plant content's connections in the MELiSSA System.

A.2.5.2 Graphics

Connections between ports of this type are represented in the model flow-sheet in brown lines.

Plants

A.2.5.3 Variables

SYMBOL	TYPE	DESCRIPTION	UNITS
C_HPc	EQUAL REAL	Relative amount of molar carbon in eatable dry part of higher plants	-
C_HPre	EQUAL REAL	Relative amount of molar carbon in dry residue of higher plants	-
f_ch_HPc	EQUAL REAL	Mass fraction of carbohydrates in edible dry part of higher plants	-
f_H2O_HPc	EQUAL REAL	Mass fraction of water in edible damp part of higher plants	-
f_H2O_HPre	EQUAL REAL	Mass fraction of water in damp residue of higher plants	-
f_lip_HPc	EQUAL REAL	Mass fraction of lipids in edible dry part of higher plants	-
f_prot_HPc	EQUAL REAL	Mass fraction of proteins in edible dry part of higher plants	-
H_HPc	EQUAL REAL	Relative amount of molar hydrogen in eatable dry part of higher plants	-
H_HPre	EQUAL REAL	Relative amount of molar hydrogen in dry residue of biomass	-
M_HPc	EQUAL REAL	Molecular weight of eatable dry part of higher plants	kg/mol
M_HPre	EQUAL REAL	Molecular weight of dry residue of higher plants	kg/mol
N_HPc	EQUAL REAL	Relative amount of molecular nitrogen in eatable dry part of higher plants	-
N_HPre	EQUAL REAL	Relative amount of molar nitrogen in dry residue of higher plants	-
Q	SUM REAL	Volumetric flow	m^3/s
O_HPc	EQUAL REAL	Relative amount of molar oxygen in eatable dry part of higher plants	-
O_HPre	EQUAL REAL	Relative amount of molar oxygen in dry residue of higher plants	-
P_HPc	EQUAL REAL	Relative amount of molar phosphorus in eatable dry part of higher plants	-
P_HPre	EQUAL REAL	Relative amount of molar phosphorus in dry residue of higher plants	-
S_HPc	EQUAL REAL	Relative amount of molar sulphur in eatable dry part of higher plants	-
S_HPre	EQUAL REAL	Relative amount of molar sulphur in dry residue of higher plants	-
W_HPc	SUM REAL	Mass flow of eatable dry part of higher plants	kg/s
W_HPre	SUM REAL	Mass flow of dry higher plants residue	kg/s

A.2.6 Port `Food`

A.2.6.1 Description

The Food Port is defining the food content's connections in the MELiSSA System.

A.2.6.2 Graphics

Connections between ports of this type are represented in the model flow-sheet in solid brown lines.

Food

A.2.6.3 Variables

SYMBOL	TYPE	DESCRIPTION	UNITS
C_ch_food	EQUAL REAL	Relative amount of molar carbon of dry food's carbohydrates	-
C_food	EQUAL REAL	Relative amount of molar carbon in dry food	-
C_lip_food	EQUAL REAL	Relative amount of molar carbon of lipids in dry food	-
C_prot_food	EQUAL REAL	Relative amount of molar carbon of proteins in dry food	-
f_ch_food	EQUAL REAL	Mass fraction of carbohydrates in dry food	-
f_H2O_food	EQUAL REAL	Mass fraction of water in damp food	-
f_lip_food	EQUAL REAL	Mass fraction of lipids in dry food	-
f_prot_food	EQUAL REAL	Mass fraction of proteins in dry food	-
H_ch_food	EQUAL REAL	Relative amount of molar hydrogen of carbohydrates in dry food	-
H_food	EQUAL REAL	Relative amount of molar hydrogen in dry food	-
H_lip_food	EQUAL REAL	Relative amount of molar hydrogen of lipids in dry food	-
H_prot_food	EQUAL REAL	Relative amount of molar hydrogen of proteins in dry food	-
M_food	EQUAL REAL	Molecular Weight of dry food	kg/mol
N_ch_food	EQUAL REAL	Relative amount of molar nitrogen of carbohydrates in dry food	-
N_food	EQUAL REAL	Relative amount of molar nitrogen in dry food	-
N_lip_food	EQUAL REAL	Relative amount of molar nitrogen of lipids in dry food	-
N_prot_food	EQUAL REAL	Relative amount of molar nitrogen of proteins in dry food	-
O_ch_food	EQUAL REAL	Relative amount of molar oxygen of carbohydrates in dry food	-
O_food	EQUAL REAL	Relative amount of molar oxygen in dry food	-
O_lip_food	EQUAL REAL	Relative amount of molar oxygen of lipids in dry food	-
O_prot_food	EQUAL REAL	Relative amount of molar oxygen of proteins in dry food	-
P_ch_food	EQUAL REAL	Relative amount of molar phosphorus of carbohydrates in dry food	-
P_food	EQUAL REAL	Relative amount of molar phosphorus in dry food	-
P_lip_food	EQUAL REAL	Relative amount of molar phosphorus of lipids in dry food	-
P_prot_food	EQUAL REAL	Relative amount of molar phosphorus of proteins in dry food	-
S_ch_food	EQUAL REAL	Relative amount of molar sulphur of	-

		carbohydrates in dry food	
S_food	EQUAL REAL	Relative amount of molar sulphur in dry food	-
S_lip_food	EQUAL REAL	Relative amount of molar sulphur of lipids in dry food	-
S_prot_food	EQUAL REAL	Relative amount of molar sulphur of proteins in dry food	-
W_food	SUM REAL	Mass flow of dry food	kg/s

A.2.7 Port `OM_edible`

A.2.7.1 Description

The OM_edible Port is defining the composition of the edible organic mater in the MELiSSA System. Thus, it does not represent a fluid stream, but information send among the subsystems that produce food.

A.2.7.2 Graphics

Connections between ports of this type are represented in the model flow-sheet in thin black lines.

OM_edible

A.2.7.3 Variables

SYMBOL	TYPE	DESCRIPTION	UNITS
C_ch	EQUAL REAL	Relative amount of molar carbon of carbohydrates	-
C_lip	EQUAL REAL	Relative amount of molar carbon of lipids	-
C_prot	EQUAL REAL	Relative amount of molar carbon of proteins	-
H_ch	EQUAL REAL	Relative amount of molar hydrogen of carbohydrates	-
H_lip	EQUAL REAL	Relative amount of molar hydrogen of lipids	-
H_prot	EQUAL REAL	Relative amount of molar hydrogen of protons	-
N_ch	EQUAL REAL	Relative amount of molar nitrogen of carbohydrates	-
N_lip	EQUAL REAL	Relative amount of molar nitrogen of lipids	-
N_prot	EQUAL REAL	Relative amount of molar nitrogen of proteins	-
O_ch	EQUAL REAL	Relative amount of molar oxygen of carbohydrates	-
O_lip	EQUAL REAL	Relative amount of molar oxygen of lipids	-
O_prot	EQUAL REAL	Relative amount of molar oxygen of proteins	-
P_ch	EQUAL REAL	Relative amount of molar phosphorus of carbohydrates	-
P_lip	EQUAL REAL	Relative amount of molar phosphorus of lipids	-
P_prot	EQUAL REAL	Relative amount of molar phosphorus of proteins	-
S_ch	EQUAL REAL	Relative amount of molar sulphur of carbohydrates	-
S_lip	EQUAL REAL	Relative amount of molar sulphur of lipids	-
S_prot	EQUAL REAL	Relative amount of molar sulphur of proteins	-

A.3 European Life Support Systems Technology Library Components

A.3.1 Compartment I - Bioreactor

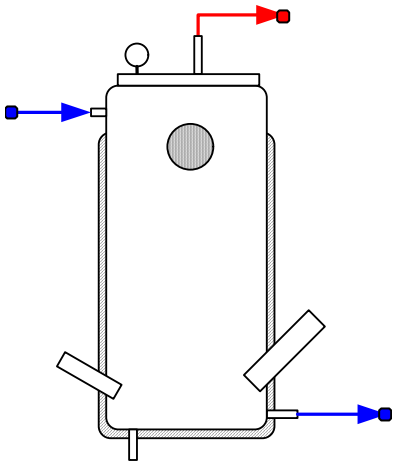
A.3.1.1 Description

This component type, named `CI_Bioreactor`, represents the liquefying compartment for biomass degradation. It has an inlet liquid fluid port that is usually connected to the biomass mixer from where it receives the residual organic matter from the whole system, as well as two outlet flow ports – one for the gas and one for the liquid produced during the anaerobic processes. More precisely, the residual biomass is degraded to volatile fatty acids (VFA), which will be further treated in Compartment II. The output products are: volatile fatty acids (acetic, propionic, butyric, valeric and caproic acids), carbon dioxide, ammonia, hydrogen, mineral salts and inert matter:

$$\text{RESIDUAL BIOMASS} \rightarrow \text{VFA} + CO_2 + NH_3 + H_2 + H_2SO_4 + H_3PO_4 + \text{INERT}$$

In the mathematical model the concentrations and volume flow rates of the outflows need to be determined, as well as the amount of non-recycled organic matter and its composition
The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.1.2 Symbol



CI_Bioreactor

A.3.1.3 Ports

Symbol	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outlet
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid inlet
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid outlet

A.3.1.4 Data

NAME	Symbol	TYPE	Default	Description	Units
$f_{H2O,Bio}$	`f H2O BIO`	REAL	0.75	Mass fraction of water in the damp biomass of the micro-organism that colonize CI	-
$h_{C,ch}$	`h_ch`	REAL	0.2	Molar fraction of C in the residue that is transformable into C of Carbohydrates	-
$h_{N,NH3}$	`h_NH3`	REAL	0.2	Molar fraction of N in the residue that is	-

				transformable into N of Ammonia	
$H_{S,H2SO4}$	h_H2SO4	REAL	0.5	Molar fraction of S in the residue that is transformable into S of H_2SO_4	-
$H_{P,H3PO4}$	h_H3PO4	REAL	0.5	Molar fraction of P in the residue that is transformable into P of H_3PO_4	-
pH	pH	REAL	6,7	pH conditions	-
Pr	Pr	REAL	$1.0132e^5$	Pressure of the reactor	Pa
R	R	REAL	8,31434	Ideal Gas Constant	(Pa m^3)/(K mol)
T	T	REAL	328	Bioreactor Temperature	K
X_{Ac}	X_Ac	REAL	0	Acetic Acid Conversion; moles of acetic acids that degrade per mole of initial acetic acids	-
X_{Bio}	X_BIO_1	REAL	0.05	Biomass conversion; moles of degraded biomass per mole of generated biomass. It is the biomass generated in the own Compartment and not the residual biomass input	-
X_{But}	X_But	REAL	0	Butyric Acid Conversion; moles of butyric acids that degrade per mole of initial butyric acids	-
X_{Cap}	X_Cap	REAL	0	Caproic Acid Conversion; moles of caproic acids that degrade per mole of initial caproic acids	-
X_{ch}	X_ch	REAL	0.8	Carbohydrate Conversion; moles of carbohydrates that degrade per mole of initial carbohydrate	-
X_{CO2}	X_CO2	REAL	0	Carbon Dioxide Conversion; moles of carbon dioxides that degrade per mole of initial Carbon Dioxide	-
X_{lip}	X_lip	REAL	0.8	Lipid Conversion; moles of lipids that degrade per mole of initial lipids	-
X_{Prop}	X_Prop	REAL	0	Propionic Acid Conversion; moles of propionic acids that degrade per mole of initial propionic acids	-
X_{prot}	X_prot	REAL	0.75	Protein Conversion; moles of proteins that degrade per mole of initial protein	-
X_{Val}	X_Val	REAL	0	Valeric Acid Conversion; moles of valeric acids that degrade per mole of initial valeric acids	-

A.3.1.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
c_i^{ionic}	Con_ionic[Compounds]	REAL	Molar concentration of the ionic forms of each compound at the liquid outlet	(mol/m^3)
c_i^{pure}	Con_pure[Compounds]	REAL	Molar concentration of the pure forms of each compound at the liquid outlet	(mol/m^3)
E_{inert}	C_inert H_inert O_inert N_inert S_inert P_inert	REAL	CHONSP Composition of inerts	-
E_{RB}	C_RB H_RB O_RB N_RB S_RB	REAL	CHONSP Relative composition of Rresidual Biomass	-

	P_RB			
E_{RB_1}	C_RB1 H_RB1 O_RB1 N_RB1 S_RB1 P_RB1	REAL	CHONSP Composition of Residual Biomass	-
E_{re}	C_re H_re O_re N_re S_re P_re	REAL	CHONSP Composition of residue	-
G_{H2CO3}	G_H2CO3	REAL	Generation of water due to the creation of carbonate in the liquid	mol/s
G_{i,BR_Cl}	G[Chemicals]	REAL	Global generation of each compound	mol/s
$G_{i,j}$	G_1[Chemicals] G_2[Chemicals] G_3[Chemicals] G_4[Chemicals] G_5[Chemicals] G_6[Chemicals] G_7[Chemicals] G_8[Chemicals] G_9[Chemicals] G_10[Chemicals] G_11[Chemicals] G_12[Chemicals]	REAL	Generation of each compound in each process	mol/s
k_i	k[Compounds]	REAL	Dissociation constant	-
M_{bio}	M_BIO_1	REAL	Molecular weight of Biomass of the microorganism that colonize the bioreactor	kg/mol
M_{inert}	M_inert	REAL	Molecular weight of inerts	kg/mol
M_m	M_prot M_lip M_ch	REAL	Molecular weight of macromolecule “m”	kg/mol
M_{RB}	M_RB	REAL	Molecular weight of Residual Biomass	kg/mol
Q_{Gout}	Qg_out	REAL	Gas volumetric outflow	m^3/s
Q_{Lout}	Ql_out	REAL	Liquid volumetric outflow	m^3/s
R	R = 8,31434	CONST REAL	Ideal gas constant	$(Pa\ m^3)/(K\ mol)$
$W_{H2O,RB,Lin}$	W_H2O_RB_in	REAL	Mass inflow of water contained in the initial Residual Biomass	kg/s
$W_{j,in}$	W_in[Compounds]	REAL	Inlet mass flow of each compound	kg/s
$W_{j,out}$	W_out[Compounds]	REAL	Outlet mass flow of each compound	kg/s
$W_{RB,Lin}$	W_RB_in	REAL	Inlet mass flow of Residual Biomass	kg/s
$W_{RB,Lout}$	W_H2O_RB_out	REAL	Mass outflow of water contained in the final Residual Biomass	kg/s
W_{RB_ND}	W_RB_ND	REAL	Mass Flow of the Residual Biomass that cannot be degraded (proteins, carbo-hydrates, lipids and inerts)	kg/s
$W_{total,in}$	W_total_in	REAL	Total inlet mass flow	kg/s
$W_{total,out}$	W_total_out	REAL	Total outlet mass flow	kg/s
$Y_{i,j}$	Y_2[Chemicals] Y_3[Chemicals] Y_4[Chemicals]	REAL	Stoichiometric coefficient of each compound in each process	-

	Y_5[Chemicals] Y_6[Chemicals] Y_7[Chemicals] Y_8[Chemicals] Y_9[Chemicals] Y_10[Chemicals] Y_11[Chemicals] Y_12[Chemicals]			
$Z_{i,Lin}$	Z_liq_in[Compounds]	REAL	Liquid inlet molar flow of each compound	mol/s
$Z_{i,Lout}$	Z_liq_out[Compounds]	REAL	Liquid outlet molar flow of each compound	mol/s
$Z_{i,Gout}$	Z_gas_out[Compounds]	REAL	Gas outlet molar flow of each compound	mol/s
$Z_{i,in}$	Z_total_in[Compounds]	REAL	Total inlet molar flow of each compound	mol/s
$Z_{i,out}$	Z_total_out[Compounds]	REAL	Total outlet molar flow of each compound	mol/s
$Z_{i,in}$	Z_in[Compounds]	REAL	Inlet molar flow of the compound	mol/s
$Z_{i,out}$	Z_out[Compounds]	REAL	Outlet molar flow of the compound	mol/s
α_i	alpha[Gas_Liquid]	REAL	Gas/liquid equilibrium constant	-
ρ_G	d_gas	REAL	Density of gas at the output	m^3/kg
ρ_L	d_liq	REAL	Density of liquid	m^3/kg

A.3.1.6 Formulation

Details on mathematical model see chapter 3.6.2

A.3.2 Compartment II - Bioreactor

A.3.2.1 Description

This component type, named `CII_Bioreactor`, represents the Photo-Heterotrophic Reactor. It has one inlet liquid fluid port that is usually connected to the outflow of Compartment I, as well as one inlet gas flow port usually also connected to the Compartment I. The two outflow ports are: a gas outflow and a liquid outflow.

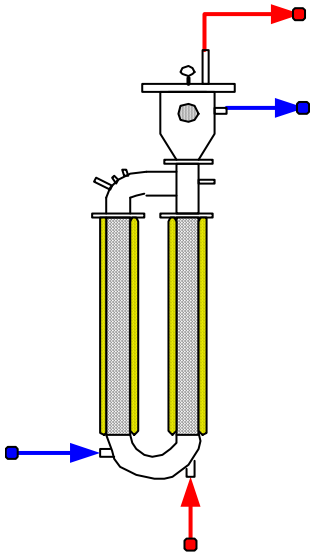
The volatile fatty acids, that are a product of Compartment I are degraded in this reactor by the use of the micro-organism *Rhodobacter Rubrum*:

$$VFA + NH_3 + H_2SO_4 + H_3PO_4 \rightarrow BIOMASS\_Rr + CO_2 + H_2O$$

Light is used as an energy source, which leads to a production of biomass, carbon dioxide and water.

The objective of the model is to obtain the concentration and volume flow rates in the output of the reactor.
The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.2.2 Symbol



CII_Bioreactor

A.3.2.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in`	Gas	(mix = Gas_Liquid)	IN	Gas inflow
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outflow
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid inflow
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid outflow

A.3.2.4 Data

NAME	SYMBOL	TYPE	DEFAULT	Description	Units

E_{m_Rr}	`C_prot`
	`H_prot`
	`O_prot`
	`N_prot`
	`S_prot`
	`P_prot`
		REAL	1
			1.5685
			0.3061
			0.2694
			$6.361e^{-3}$
				RelativeComposition of the macromolecule "m" of *R. Rubrum*; the moles of the element E per each mole of the macromolecule "m" The value is according to:	-

	C_lip H_lip O_lip N_lip S_lip P_lip C_ch H_ch O_ch N_ch S_ch P_ch C_RNA H_RNA O_RNA N_RNA S_RNA P_RNA C_DNA H_DNA O_DNA N_DNA S_DNA P_DNA		0 1 1.0223 0.2153 0 0 0.263 1 1.5405 0.5135 0 0 0 1 1.2295 0.7256 0 0 0.1043 1 1.2585 0.6205 0.3961 0 1.034	$(CH_{1.5685}O_{0.3061}N_{0.2694}S_{0.006361})_{prot}$ $(CH_{1.9223}O_{0.2153})_{lip}$ $(CH_{1.5405}O_{0.5135})_{ch}$ $(CH_{1.2295}O_{0.7256}P_{0.1043})_{RNA}$ $(CH_{1.2585}O_{0.6205}N_{0.3961}P_{1.034})_{DNA}$	
f_{m_Rr}	f_prot_Rr f_lip_Rr f_ch_Rr f_RNA_Rr f_DNA_Rr f_H2O_Rr	REAL	0.6106 0.216 0.1171 0.0365 0.0198 0.75	Mass fraction of the macromolecule "m_Rr" in the dry biomass of *R. Rubrum*	-
pH	pH	REAL	6,9	pH conditions	-
Pr	Pr	REAL	$1.0132e^5$	Pressure	Pa
T	T	REAL	303	Bioreactor Temperature	K
X_{VFA}	X_ac X_prop X_but X_val X_cap	REAL	1 1 1 0.95 0.95	Conversion of each VFA; the moles of VFA reacting per mole of initial VFA	-

A.3.2.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
c_i^{ionic}	Con_ionic[Compounds]	REAL	Molar concentration of the ionic forms of each compound at the liquid outlet	(mol/m^3)
c_i^{pure}	Con_pure[Compounds]	REAL	Molar concentration of the pure forms of each compound at the liquid outlet	(mol/m^3)

E_{m_Rr}	C[m_Rr] H[m_Rr] O[m_Rr] N[m_Rr] S[m_Rr] P[m_Rr]	REAL	CHONSP Relative composition of Macromolecules m in dry R. rubrum biomass	-
E_{Rr}	C_Rr H_Rr O_Rr N_Rr S_Rr P_Rr	REAL	Relative composition of dry biomass of R. Rubrum. Mols of each element per mol of R. rubrum	-
E_{Rr_1}	C_Rr1 H_Rr1 O_Rr1 N_Rr1 S_Rr1 P_Rr1	REAL	Composition of dry biomass of R. Rubrum	-
f_{m_Rr}	f[m_Rr]	REAL	Mass fraction of the macromolecule "m_Rr" in dry biomass of R. Rubrum	-
G_{H2CO3}	G_H2CO3	REAL	Generation of water due to the creation of carbonate in the liquid	mol/s
G_i	G[Compounds]	REAL	Global generation of each compound	mol/s
$G_{i,j}$	G_14[Compounds] G_15[Compounds] G_16[Compounds] G_17[Compounds] G_18[Compounds]	REAL	Generation of each compound in each process	mol/s
k_i	k[Compounds]	REAL	Dissociation constant	-
M_{m_Rr}	M_m_Rr[m_Rr]	REAL	Molecular weight of macromolecules “m_Rr” in R. rubrum biomass	kg/mol
M_{Rr}	M_Rr	REAL	Molecular weight of R. rubrum dry biomass	kg/mol
Q_{Gout}	Qg_out	ALG REAL	Gas volumetric outflow	m^3/s
Q_{Lout}	Ql_out	ALG REAL	Liquid volumetric outflow	m^3/s
R	R = 8,31434	CONST REAL	Ideal gas constant	(Pa m^3)/(K mol)
$W_{i,in}$	W_in[Compounds]	REAL	Inlet mass flow of each compound	kg/s
$W_{j,out}$	W_out[Compounds]	REAL	Outlet mass flow of each compound	kg/s
$w_{total,in}$	W_total_in	REAL	Total inlet mass flow	kg/s
$w_{total,out}$	W_total_out	REAL	Total outlet mass flow	kg/s
$Y_{i,j}$	Y_14[Chemicals] Y_15[Chemicals] Y_16[Chemicals] Y_17[Chemicals] Y_18[Chemicals]	REAL	Stoichiometric coefficient of each compound for each process	-
$Z_{i,Gin}$	Z_gas_in[Compounds]	REAL	Gas inlet molar flow of each compound	mol/s
$Z_{i,Gout}$	Z_gas_out[Compounds]	REAL	Gas outlet molar flow of each compound	mol/s
$Z_{i,Lin}$	Z_liq_in[Compounds]	REAL	Liquid inlet molar flow of each compound	mol/s
$Z_{i,Lout}$	Z_liq_out[Compounds]	REAL	Liquid outlet molar flow of each compound	mol/s
$Z_{i,in}$	Z_total_in[Compounds]	REAL	Total inlet molar flow of each	mol/s

			compound	
$Z_{i,out}$	`Z_total_out[Compounds]`	REAL	Total outlet molar flow of each compound	mol/s
α_i	`alpha[Gas_Liquid]`	REAL	Gas/liquid equilibrium constant	-
ρ_G	`d_gas`	REAL	Density of gas	m^3/kg
ρ_L	`d_liq`	REAL	Density of liquid	m^3/kg

A.3.2.6 Formulation

Details on mathematical model see chapter 3.6.3

A.3.3 Compartment III - Bioreactor

A.3.3.1 Description

This component type, named `CIII_Bioreactor`, represents the nitrifying reactor. It has one inlet liquid fluid port that is usually connected to the outflow of compartment II, as well as one inlet gas flow port usually receiving gas from the gas treatment unit. The two outflow ports are: a gas outflow and a liquid outflow.

Compartment III has the function to transform ammonia into nitrate which will be used as nutrient for the autotrophy organisms. It is an aerobic process carried out by *Nitrosomonas europaea* and *Nitrobacter winogradskyi* micro-organisms.

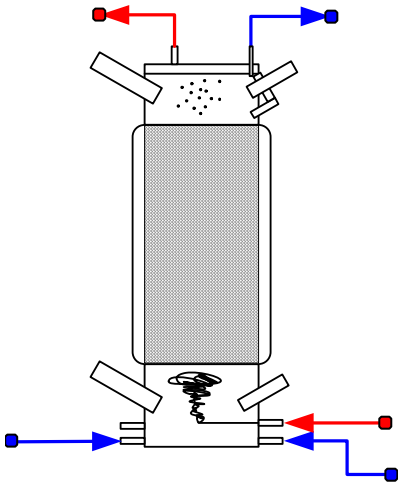
$$O_2 + CO_2 + NH_3 + H2SO4 + H_3PO_4 \rightarrow BIOMASS\_3 + HNO_3 + H_2O$$

N. eurepaea and *N. winogradkyi* biomass must be removed from the reactor to avoid their decay and the production of unwanted substrates as well as to be able to work at steady state.

The objective of the mathematical model is to gain the concentration and volume flow rates of these outputs.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.3.2 Symbol



CIII_Bioreactor

A.3.3.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in`	Gas	(mix = Gas_Liquid)	IN	Gas inflow
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outflow
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid inflow
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid outflow

A.3.3.4 Data

NAME	SYMBOL	TYPE	DEFAULT	Description	Units

E_{New}	`C_New`
	`H_New`
	`O_New`
	`N_New`
	`S_New`
		REAL	1
			1.6147
			0.3906
			0.1994
				Relative composition of N. Eurepaea and N. Winogradkyi. Fixed data, with a fixed stoichoimetry.	-

	P_New		0.0035 0.0089		
$f_{H2O,\ New}$	f_H2O_New	REAL	0.75	Mass fraction of water in the damp biomass	-
f_{m_New}	f_prot_New f_lip_New f_ch_New	REAL	0.52559 0.1993 0.1444	Mass fraction of biological macromolecules "m_New" in the dry biomass	-
Pr	Pr	REAL	$1.0132e^{5}$	Pressure of the reactor	Pa
pH	pH	REAL	8,1	pH conditions	-
T	T	REAL	302	Bioreactor Temperature	K
Tm_{Ne}	Tm_Ne	REAL	0.76	Maintenance of Nitrobacter. This is the molar fraction of oxidized to nitrite maintaining the Nitrobacter bacteria.	-
Tm_{Nw}	Tm_Nw	REAL	0.81	Maintenance of Nitrosomonas. The molar fraction of oxidized ammonia maintaining Nitrosomonas bacteria.	-
X_{HNO2}	X_HNO2	REAL	1	Conversion of nitrite. The moles of nitrite that assimilates the Nitrobacters per mole of initial nitrite.	-
X_{NH3}	X_NH3	REAL	0.85	Conversion of ammonia. The moles of ammonia that assimilates the Nitrosomonas per mole of initial ammonia.	-
X_{urea}	X_urea	REAL	1	Conversion of urea. The moles of urea that are transformed into carbon dioxide and ammonia per mole of initial urea.	-
X_{uric}	X_uric	REAL	1	Conversion of uric acid. The moles of uric acid that are transformed into carbon dioxide and ammonia per mole of initial uric acid.	-

A.3.3.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
c_i^{ionic}	Con_ionic[Compounds]	REAL	Molar concentration of the ionic forms of each compound at the liquid outlet	mol/m^3
c_i^{pure}	Con_pure[Compounds]	REAL	Molar concentration of the pure forms of each compound at the liquid outlet	mol/m^3
fv_{Lin}	fv_liq	REAL	Volumetric fraction of liquid in the total liquid inflow	-
fv_{urine}	fv_urine	REAL	Volumetric fraction of urine in the total liquid inflow	-
$G_{HNO2,j}$	G_19_HNO2 G_20_HNO2 G_21_HNO2 G_22_HNO2	REAL	Generation of nitrite for each process related to the nitrification	mol/s
$G_{i,j}$	G_19[Compounds] G_20[Compounds] G_21[Compounds] G_22[Compounds]	REAL	Generation of each compound for each process related to the nitrification	mol/s
G_{HNO2}	G_HNO2	REAL	Global generation of nitrite	mol/s
G_{H2CO3}	G_H2CO3	REAL	Generation of water due to the creation of carbonate in the liquid	mol/s
G_i	G[Compounds]	REAL	Global generation of each compound	mol/s
G_{Ne_HNO2}	G_Ne_NH3	REAL	Generation of ammonia due to the assimilation of Nitrosomonas	mol/s
G_{Nw_HNO2}	G_Nw_HNO2	REAL	Generation of nitrite due to the assimilaton of Nitrobacters	mol/s
k_i	k[Compounds]	REAL	Dissociation constant	-
M_{New}	M_New	REAL	Molecular weight of New biomass	kg/mol

Q_{Gout}	Qg_out	ALG REAL	Gas volumetric outflow	m^3/s
Q_{Lout}	Ql_out	ALG REAL	Liquid volumetric outflow	m^3/s
R	R = 8,31434	CONST REAL	Ideal gas constant	(Pa m^3)/(K mol)
$W_{j,in}$	W_in[Compounds]	REAL	Inlet mass flow of each compound	kg/s
$W_{j,out}$	W_out[Compounds]	REAL	Outlet mass flow of each compound	kg/s
$w_{total,in}$	W_total_in	REAL	Total inlet mass flow	kg/s
$w_{total,out}$	W_total_out	REAL	Total outlet mass flow	kg/s
$Y_{HNO2,j}$	Y_19_HNO2 Y_20_HNO2 Y_21_HNO2 Y_22_HNO2	REAL	Stoichiometric coefficient of nitrite for each process related to the nitrification	
$Y_{i,j}$	Y_19[Chemicals] Y_20[Chemicals] Y_21[Chemicals] Y_22[Chemicals]	REAL	Stoichiometric coefficient of each compound for each process related to the nitrification	-
$Z_{i,Gin}$	Z_gas_in[Compounds]	REAL	Gas inlet molar flow of each compound	mol/s
$Z_{i,Gout}$	Z_gas_out[Compounds]	REAL	Gas outlet molar flow of each compound	mol/s
$Z_{i,Lin}$	Z_liq_in[Compounds]	REAL	Liquid inlet molar flow of each compound	mol/s
$Z_{i,Lout}$	Z_liq_out[Compounds]	REAL	Liquid outlet molar flow of each compound	mol/s
$Z_{i,in}$	Z_total_in[Compounds]	REAL	Total inlet molar flow of each compound	mol/s
$Z_{i,out}$	Z_total_out[Compounds]	REAL	Total outlet molar flow of each compound	mol/s
α_i	alpha[Compounds]	REAL	Gas/liquid equilibrium constant	-
ρ_G	d_gas	REAL	Density of gas at outlet	kg/m^3
ρ_{Lin}	d_liq_in	REAL	Density of liquid at outline	kg/m^3
ρ_{Lout}	d_liq	REAL	Density of liquid at inline	kg/m^3
ρ_{urine}	d_urine_in	REAL	Density of urine at inline	kg/m^3

A.3.3.6 Formulation

Details on mathematical model see chapter 3.6.4

A.3.4 Compartment IVa - Bioreactor

A.3.4.1 Description

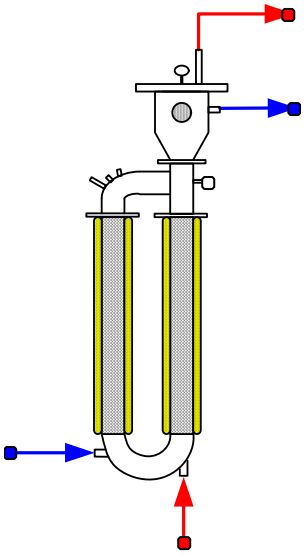
This component type, named `CIVa_Bioreactor`, represents the photosynthetic compartment. It has one inlet liquid fluid port that is usually connected via a solid-liquid separator and a liquid distributor with Compartment III, as well as one inlet gas flow port. The two outflow ports are: a gas outflow and a liquid outflow. The liquid outflow contains the eatable biomass that will be further treated before being sent to the crew compartment.

This bioreactor has the objective to generate edible biomass by means of a photosynthetic process. Thus, compartment IVa is able to produce edible biomass, the algae species *Arthrospira platensis* and oxygen by using the basic nutrients (phosphates, sulphates and nitrates), carbon dioxide as a carbon source and light as energy source,.

$$HNO_3 + H_2SO_4 + H_3PO_4 + CO_2 \rightarrow BIOMASS\_4a + O_2 + H_2O$$

The mathematical model has a gas and liquid inlet and a gas and liquid output. It is designed to determine the concentrations and volume flow rates of the outputs from the bioreactor.
The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.4.2 Symbol



CIVa_Bioreactor

A.3.4.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in`	Gas	(mix = Gas_Liquid)	IN	Gas inflow
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outflow
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid inflow
`liq_out`	Liquid	mix = Compounds)	OUT	Liquid outflow
sensor	OM_edible		OUT	Sensor about composition

A.3.4.4 Data

NAME	SYMBOL	TYPE	DEFAULT	Description	Units

E_{m_Ap}	`C_prot`
	`H_prot`
	`O_prot`
	`N_prot`
	`S_prot`
		REAL	1
			1.526
			0.327
			0.2496
				Relative composition of biological macromolecules "m_Ap" comprising of Arthrospira. The moles of each element of the macromolecule "m_Ap" for each mole of	-

	P_prot C_lip H_lip O_lip N_lip S_lip P_lip C_ch H_ch O_ch N_ch S_ch P_ch C_ex H_ex O_ex N_ex S_ex P_ex C_DNA H_DNA O_DNA N_DNA S_DNA P_DNA		0 0 1 1.714 0.204 0 0 0 1 1.670 0.711 0 0 0 1 1.650 0.950 0 0 0 1 1.273 0.701 0.393 0 0	macromolecule "m_Ap".	
$f_{H2O,\ Ap}$	f_H2O_Ap	REAL	0.75	Mass fraction of water in the damp *Arthrospira* biomass	-
F_o	Fo	REAL	94.37	Light intensity	W / m^2
pH	pH	REAL	9.5	pH conditions	-
Pr	Pr	REAL	$1.01325e^5$	Pressure	Pa
T	T	REAL	309	Bioreactor Temperature	K
X_{HNO3}	X_HNO3	REAL	0.95	Conversion of nitrate. The moles of nitrate reacting per mole of initial nitrate	-

A.3.4.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
c_i^{ionic}	Con_ionic[Compounds]	REAL	Molar concentration of the ionic forms of each compound at the liquid outlet	mol/m^3
c_i^{pure}	Con_pure[Compounds]	REAL	Molar concentration of the pure forms of each compound at the liquid outlet	mol/m^3
E_{Ap}	C_Ap H_Ap O_Ap N_Ap S_Ap P_Ap	REAL	Relative CHONSP composition of dry biomass of A. platensis.	-
E_{Ap_1}	C_Ap1 H_Ap1 O_Ap1 N_Ap1 S_Ap1 P_Ap1	REAL	CHONSP Composition of dry biomass of A. platensis	-
E_{m_Ap}	C[m_Ap]	REAL	Relative CHONSP composition of	-

	H[m_Ap] O[m_Ap] N[m_Ap] S[m_Ap] P[m_Ap]		biological macromolecules "m_Ap" comprising of A. platensis	
f_{m_Ap}	f[m_Ap]	REAL	Mass fraction of the macromolecule "m_Ap" in dry biomass of A. platensis	-
G_{H2CO3}	G_H2CO3	REAL	Generation of water due to the creation of carbonate in the liquid	mol/s
G_i	G[Compounds]	REAL	Global generation	mol/s
k_i	k[Compounds]	REAL	Dissociation constant	-
M_{Ap}	M_Ap	REAL	Molecular weight of dry biomass of A. platensis	kg/mol
M_{m_Ap}	M_m_Ap[m_Ap]	REAL	Molecular weight of macromolecules “m_Ap” in dry A. platensis biomass	kg/mol
Q_{Gout}	Qg_out	ALG REAL	Gas volumetric outflow	m^3/s
Q_{Lout}	Ql_out	ALG REAL	Liquid volumetric outflow	m^3/s
R	R = 8,31434	CONST REAL	Ideal gas constant	(Pa m^3)/(K mol)
$W_{j,in}$	W_in[Compounds]	REAL	Inlet mass flow of each compound	kg/s
$W_{j,out}$	W_out[Compounds]	REAL	Outlet mass flow of each compound	kg/s
$w_{total,in}$	W_total_in	REAL	Total inlet mass flow	kg/s
$w_{total,out}$	W_total_out	REAL	Total outlet mass flow	kg/s
$Z_{i,Gin}$	Z_gas_in[Compounds]	REAL	Gas inlet molar flow of each compound	mol/s
$Z_{i,Gout}$	Z_gas_out[Compounds]	REAL	Gas outlet molar flow of each compound	mol/s
$Z_{i,Lin}$	Z_liq_in[Compounds]	REAL	Liquid inlet molar flow of each compound	mol/s
$Z_{i,Lout}$	Z_liq_out[Compounds]	REAL	Liquid outlet molar flow of each compound	mol/s
$Z_{i,in}$	Z_total_in[Compounds]	REAL	Total inlet molar flow of each compound	mol/s
$Z_{i,out}$	Z_total_out[Compounds]	REAL	Total outlet molar flow of each compound	mol/s
$Y_{i,j}$	Y_23[Compounds]	REAL	Stoichiometric coefficient of each compound in the photosynthetic process	-
α_i	alpha[Gas_Liquid]	REAL	Gas/liquid equilibrium constant	-
ρ_G	d_gas	REAL	Density of gas	m^3/kg
ρ_L	d_liq	REAL	Density of liquid	m^3/kg

A.3.4.6 Formulation

Details on mathematical model see chapter 3.6.5

A.3.5 Compartment IVb – Higher Plants Chamber

A.3.5.1 Description

This component type, named `Higher_Plants_Chamber`, represents the Higher Plants Chamber (HPC). The information from the `Plants_Composition` component described in section A.3.7 is integrated into this component.

`Higher_Plants_Chamber` component has one inlet liquid fluid port that is usually connected via a solid-liquid separator and a liquid divisor with compartment III, as well as one inlet gas flow port. The three outflow ports are: a gas outflow, a liquid outflow and a solid output. The solid output corresponds to the higher plants, while the liquid output is the liquid surplus of the chamber. The gas output is for the produced oxygen.

The function of the HPC is the provision of life support elements including mainly food production, but also CO_2 fixation, O_2 generation and potable water production.

The process that takes place is very similar to the process in compartment IVa, since both are a photosynthetic process. Thus, plants use the basic nutrients as nitrogen, sulphur and phosphor source, CO_2 as carbon source and light as energy source in order to produce biomass:

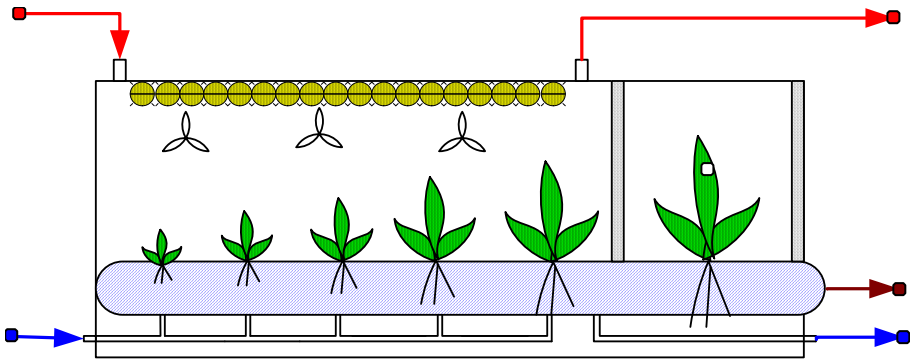
$$HNO_3 + H_2SO_4 + H_3PO_4 + HNO_3 + NH_3 + CO_2 + H_2O \rightarrow BIOMASS\_4b + O_2$$

The plants composition (macromolecule mass fraction and composition) has been build up by a pool of 8 plants: tomato, potatoes, salad, wheat, rice, soybean, onion and spinach.

The model's objective is to calculate the concentration and the volumetric flows at the outlet, the CHONSP composition of the global biomass produced (differentiated between edible and non edible), the required area for the production of each crop, as well as the total required area. The BR_CIVa is assumed to be constantly illuminated so that the plants are constantly doing photosynthesis.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.5.2 Symbol



Higher_Plants_Chamber

A.3.5.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in`	Gas	(mix = Gas_Liquid)	IN	Gas inflow
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid inflow
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outflow
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid outflow
`plant`	solid	(mix = Compounds)	OUT	Plant outflow

sensor	OM_edible		OUT	Sensor about composition

A.3.5.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
$(f_{com,com})_v$	f_tomato f_potato f_wheat f_rice f_salad f_soybean f_onion f_spinach	REAL	0.008 0.295 0.483 0.161 0.005 0.016 0.016 0.016	Mass fraction of the dry edible part of a plant "v" in total edible biomass	-
$(f_{HNO3,NH3})_v$	f_HNO3_tomato f_HNO3_potato f_HNO3_wheat f_HNO3_rice f_HNO3_salad f_HNO3_soybean f_HNO3_onion f_HNO3_spinach	REAL	5 5 5 5 5 5 5 5	kg of HNO3 per kg of NH3 for each plant "v"	-
Pr	Pr	REAL	$1.01325e^5$	Chamber Pressure	Pa
T	T	REAL	298	Chamber Temperature	K
W_{com}	W_HPc_total	REAL	$2e^{-6}$	Quantity of total edible biomass to be produced (in dry weight)	kg/s

A.3.5.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
A_{total}	A_total	REAL	Total harvesting area	m^2
A_v	A[Crops]	REAL	Harvesting area per plant species	m^2
$E_{m\_HPc\_1}$	C1_ch_HPc H1_ch_HPc O1_ch_HPc N1_ch_HPc S1_ch_HPc P1_ch_HPc Analogue for: Proteins (prot) Lipids (lip)	REAL	CHONSP composition of carbohydrates of eatable parts ofhigher plants	-
$E_{com,v}$	C_HPc[Crops] H_HPc[Crops] O_HPc[Crops] N_HPc[Crops] S_HPc[Crops] P_HPc[Crops]	REAL	Relative CHONSP composition of biomass of eatable dry part of each plant species	-
$E_{com\_1,v}$	C_HPc1[Crops] H_HPc1[Crops] O_HPc1[Crops] N_HPc1[Crops] S_HPc1[Crops] P_HPc1[Crops]	REAL	CHONSP composition of biomass of eatable dry part of each plant species	-
E_{HPc_1}	C_HPc1_total H_HPc1_total O_HPc1_total N_HPc1_total S_HPc1_total P_HPc1_total	REAL	CHONSP composition of overall biomass of eatable part of higher plants	-
E_{HPre_1}	C_HPre1 H_HPre1 O_HPre1 N_HPre1	REAL	CHONSP composition of biomass of non-eatable part of higher plants	-

	S_HPre1 P_HPre1			
E_v	C_plant[Crops] H_plant[Crops] O_plant[Crops] N_plant[Crops] S_plant[Crops] P_plant[Crops]	REAL	Relative CHONSP composition of each higher plant (waste + eatable)	-
E_{v_1}	C_plant1[Crops] H_plant1[Crops] O_plant1[Crops] N_plant1[Crops] S_plant1[Crops] P_plant1[Crops]	REAL	CHONSP composition of each higher plant (waste + eatable)	-
$(f_{com,com})_v$	f[Crops]	REAL	Mass Fraction of plant species	-
$G_{i,G}$	G_gas[Gas_Liquid]	REAL	Generation of each compound in gas phase	mol/s
$G_{i,HPC}$	G[Compounds]	REAL	Global generation of each compound	mol/s
$G_{i,L}$	G_liq[Compounds]	REAL	Generation of each compound in liquid phase	mol/s
$(G_{i,HPC})_v$	G1[Compounds] G2[Compounds] G3[Compounds] G4[Compounds] G5[Compounds] G6[Compounds] G7[Compounds] G8[Compounds]	REAL	Generation of each compound to produce the plant "v"	mol/s
$M_{v,com}$	M_HPc[Crops]	REAL	Molecular weight of each eatable dry plant "v"	kg/mol
M_v	M_plant[Crops]	REAL	Molecular weight of each dry plant	kg/mol
R	R = 8,31434	CONST REAL	Ideal gas constant	(Pa m^3)/(K mol)
W_v	W[Crops]	REAL	Mass flow of each dry plant "v"	kg/s
$W_{re,v}$	W_HPre[Crops]	REAL	Mass flow of the dry residual part of each plant "v"	kg/s
$W_{com,v}$	W_HPc[Crops]	REAL	Mass flow of the dry eatable part of each plant "v"	kg/s
$W_{H2O,HPc}$	W_H2O_HPc[Crops]	REAL	Mass flow of water contained in the damp eatable part of each plant "v"	kg/s
$W_{H2O,HPre}$	W_H2O_HPre[Crops]	REAL	Mass flow of water contained in the damp residual part of each plant "v"	kg/s
$W_{H2O,trans}$	W_H2O_trans[Crops]	REAL	Mass flow of water transpired by each plant "v"	kg/s
$W_{H2O,v}$	W_H2O[Crops]	REAL	Mass flow of water contained in each plant "v"	kg/s
$W_{H2O,HPc}$	W_H2O_HPc_total	REAL	Total mass flow of water contained in the total biomass of the eatable part	kg/s
$W_{H2O,HPre}$	W_H2O_HPre_total	REAL	Total mass flow of water contained in the total biomass of the residual part	kg/s
$W_{H2O,HP}$	W_H2O_HP	REAL	Total mass flow of water contained in the total biomass of the higher plants	kg/s
$W_{H2O,trans}$	W_H2O_trans_HP	REAL	Total mass flow of water transpired by the higher plants	kg/s
$(Y_{i,HPC})_v$	Y1[Compounds] Y2[Compounds] Y3[Compounds] Y4[Compounds] Y5[Compounds] Y6[Compounds] Y7[Compounds] Y8[Compounds]	REAL	Stoichiometric coefficients of each compound in each process (to produce each plant specie)	-

$(Y_{v,HPC})_v$	Y1_tomato Y2_potato Y3_wheat Y4_rice Y5_salad Y6_soybean Y7_onion Y8_spinach	REAL	Stoichiometric coefficients of each plant specie	-
$Z_{H2O,HP}$	Z_H2O_content_HP	REAL	Molar flow of water in the higher plants biomass	mol/s
$Z_{i,Lin}$	Z_liq_in[Compounds]	REAL	Molar liquid inflow of each compound	mol/s
$Z_{i,Gin}$	Z_gas_in[Compounds]	REAL	Molar gaseous inflow of each compound	mol/s
$Z_{i,Lout}$	Z_liq_out[Compounds]	REAL	Molar liquid inflow of each compound	mol/s
$Z_{i,Gout}$	Z_gas_out[Compounds]	REAL	Molar gaseous inflow of each compound	mol/s
ρ_L	d_liq	REAL	Density of liquid	m^3/kg

A.3.5.6 Formulation

Details on mathematical model see chapter 3.7.1

A.3.6 Compartment V – Crew Compartment

A.3.6.1 Description

This component type, named `Crew_Compartment`, receives food, oxygen and water and transform it to faeces, urine and metabolism products (water and carbon dioxide).

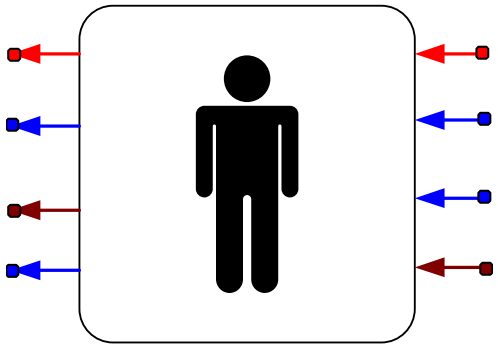
$$FOOD + O_2 + WATER \rightarrow FAECES + URINE + CO_2 + H_2O$$

It has one inlet solid port that is usually connected to the food treatment unit, an inlet gas port that usually comes from the photosynthetic subsystems and supports the chamber with a breathable atmosphere, as well as two inlet water flow port – one for hygienic and one for potable water. The four outflow ports are: a gas outflow, a liquid outflow, a urine outflow and a solid output (faeces).

The model objective is to obtain the concentration and the volumetric flows at the outlet. One of the assumptions in the model is that anabolism and catabolism are in dynamic equilibrium. Consequently, there is no accumulation, which means that the crew neither gains nor looses weight.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.6.2 Symbol



Crew_Compartment

A.3.6.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`Food`	Food		IN	Food inflow
`gas_in`	Gas	(mix = Gas_Liquid)	IN	Gas inflow
`hyg_water`	Liquid	(mix = Water)	IN	Hygiene water inflow
`potable_water`	Liquid	(mix = Water)	IN	Potable water inflow
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outflow
`liq_urine`	Liquid	(mix = Urine_compounds)	OUT	Urine outflow
`liq_water_out`	Liquid	(mix = Water)	OUT	Residual water outflow
`solid_out`	Solid	(mix = Compounds)	OUT	Faeces outflow

A.3.6.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS

$f(Abs)_m$	`f_abs_prot`
	`f_abs_lip`
	`f_abs_ch`
		REAL	0.95
			0.90
			0.99
				Mass fraction of each macro-molecule “m” that is absorbed inside the human body	-

$f_{cre,\ urine}$	f_creat_su	REAL	0.042	Fraction mass creatinine in the urine (in dry weight)	-
$(f_{H2O})_{fc}$	f_H2O_Fc	REAL	0.08	Mass fraction of water contained in faeces in correspondence to the water contence in the human body	-
$(f_{H2O})_{persp}$	f_H2O_persp	REAL	0.25	Mass fraction of perspirated water contained in urine in correspondence to the water contence in the human body	-
$(f_{H2O})_{resp}$	f_H2O_resp	REAL	0.17	Mass fraction of breathable water in correspondence to the water contence in the human body	-
$(f_{H2O})_{urine}$	f_H2O_urine	REAL	0.5	Mass fraction of water contained in urine in correspondence to the water contence in the human body	-
$f_{urea,\ urine}$	f_urea_su	REAL	0.51	Mass fraction of urea in the urine (in dry weight)	-
$f_{ureic,\ urine}$	f_ureic_su	REAL	0.014	Mass fraction of ureic acid in the urine (dry weight)	-
Pr	Pr	REAL	101325e[5]	Pressure	Pa
T	T	REAL	298	Chamber Temperature	K
$\%(H_2O)_d$	f_H2O_WC_faeces f_H2O_WC_urine f_H2O_shower	REAL	0.1 0.1 0.8	Fraction of hygienic water necessary for destination “d” (flush water for faeces, flush water for urine, shower water)	-

A.3.6.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
E_{fc}	C_Fc H_Fc O_Fc N_Fc S_Fc P_Fc	REAL	Relative CHONSP composition of Faeces (in dry weight)	-
E_{fc_1}	C_faeces1 H_faeces1 O_faeces1 N_faeces1 S_faeces1 P_faeces1	REAL	CHONSP composition of faeces (in dry weight)	-
E_{SU}	C_solid_urine H_solid_urine O_solid_urine N_solid_urine S_solid_urine P_solid_urine	REAL	Relative CHONSP composition of solid urine	-
E_{SU_1}	C1_solid_urine H1_solid_urine O1_solid_urine N1_solid_urine S1_solid_urine P1_solid_urine	REAL	CHONSP composition of solid urine	-
E_{urine_1}	C_urine1 H_urine1 O_urine1 N_urine1 S_urine1 P_urine1	REAL	CHONSP composition of urine (in dry weight)	-
$G_{i,CC}$	G25[Chemicals]	REAL	Global generation of each compound	mol/s

$G_{food,CC}$	G25_food	REAL	Global generation of food	mol/s
M_{fc}	M_Fc	REAL	Molecular weight of faeces (in dry weight)	kg/mol
$M_{m,ing}$	M_prot_abs M_lip_abs M_ch_abs	REAL	Molecular weight of each macromolecules of ingested food (in dry weight)	kg/mol
M_{SU}	M_solid_urine	REAL	Molecular weight of solid urine	kg/mol
$Q_{H2O,body}$	Q_water_body	REAL	Volumetric flow of the water body	m^3/s
$Q(H2O)_d$	Q_water_WC_faeces Q_water_WC_urine Q_water_drink Q_water_hygiene	REAL	Volumetric flow of the water necessary for destination “d” (flush water for faeces, flush water for urine, drink water and shower water)	m^3/s
R	R = 8,31434	CONST REAL	Ideal gas constant	(Pa m^3)/(K mol)
$W_{m,abs}$	W_prot_abs W_lip_abs W_ch_abs	REAL	Mass flow of absorbed macromolecules	kg/s
$W_{m,fc}$	W_prot_faeces W_lip_faeces W_ch_faeces	REAL	Mass flow of macromolecules contained in faeces	kg/s
$W_{m,food}$	W_prot_food W_lip_food W_ch_food	REAL	Mass flow of macromolecules contained in food	kg/s
Derived from V.24	W_H2O_gas	REAL	Mass flow of water in gaseous phase	kg/s
$W_{H2O,fc}$	W_H2O_Fc	REAL	Mass flow of water contained in faeces	kg/s
W_{fc}	W_Fc	REAL	Mass flow of faeces (in dry weight)	kg/s
$Z_{i,urine}$	Z[Urine_compounds]	REAL	Molar flow of each compound of urine	mol/s
$Z_{i,Gin}$	Z_gas_in[Compounds]	REAL	Molar gas inflow of each compound	mol/s
$Z_{i,Gout}$	Z_gas_out[Compounds]	REAL	Molar gas outflow of each compound	mol/s

A.3.6.6 Formulation

Details on mathematical model see chapter 3.7.2

A.3.7 Plants Composition

A.3.7.1 Description

This component type, named `Plants_Composition`, gathers the data about the plants' composition needed for the `Higher_Plants` component.

As this component represents only collection data, there is no symbol and no ports.

A.3.7.2 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
$E_{m\_HPc,v}$	C_prot_soybean H_prot_soybean O_prot_soybean N_prot_soybean S_prot_soybean P_prot_soybean C_lip_sat_soybean H_lip_sat_soybean O_lip_sat_soybean N_lip_sat_soybean S_lip_sat_soybean P_lip_sat_soybean C_lip_insat_soybean H_lip_insat_soybean O_lip_insat_soybean N_lip_insat_soybean S_lip_insat_soybean P_lip_insat_soybean C_ch_soybean H_ch_soybean O_ch_soybean N_ch_soybean S_ch_soybean P_ch_soybean C_fib_soybean H_fib_soybean O_fib_soybean N_fib_soybean S_fib_soybean P_fib_soybean C_ARN_soybean H_ARN_soybean O_ARN_soybean N_ARN_soybean S_ARN_soybean P_ARN_soybean C_DNA_soybean H_DNA_soybean O_DNA_soybean N_DNA_soybean S_DNA_soybean P_DNA_soybean Analogue for: tomato potato wheat rice salad	REAL	*)	Relative composition of macromolecules "m_HPc" of the higher plants "v"	-

	onion spinach				
$E_{re,v}$	C_HPre_soybean H_HPre_soybean O_HPre_soybean N_HPre_soybean S_HPre_soybean P_HPre_soybean Analogue for: tomato potato wheat rice salad onion spinach	REAL	*)	Composition of the residue from the plant "v" in moles of the element (CHONSP) of the residue per mole of residue	-
CY_v	CY_tomato CY_potato CY_wheat CY_rice CY_salad CY_soybean CY_onion CY_spinach	REAL	*)	Crop yield of harvested plant “v” (in dry weight)	$(kg)_{v\ dried}$ / (m^2s)
$(f_{H2O,com})_v$	f_H2O_c_tomato f_H2O_c_potato f_H2O_c_wheat f_H2O_c_rice f_H2O_c_salad f_H2O_c_soybean f_H2O_c_onion f_H2O_c_spinach	REAL	*)	Mass fraction of water in damp edible part of higher plant’s “v” biomass	-
$(f_{H2O,re})_v$	f_H2O_re_tomato f_H2O_re_potato f_H2O_re_wheat f_H2O_re_rice f_H2O_re_salad f_H2O_re_soybean f_H2O_re_onion f_H2O_re_spinach	REAL	*)	Mass fraction of water in damp residual biomass of higher plants “v”	-
$(f_{m\_HPc,com})_v$	f_prot_soybean f_lip_soybean f_lip_sat_soybean f_ch_soybean f_RNA_soybean f_DNA_soybean Analogue for: tomato potato wheat rice salad onion spinach	REAL	*)	Mass fraction of macromolecules "m_HPc" on the dry mass of comestible higher plants "v"	-
$(f_{re,com})_v$	f_re_tomato f_re_potato f_re_wheat f_re_rice f_re_salad f_re_soybean f_re_onion f_re_spinach	REAL	*)	Mass fraction of the residual portion of the plant in the edible portion of the plant "v” in kilograms of waste per kg of edible plant "v" (dry weight)	-
TW_v	TW_tomato TW_potato TW_wheat TW_rice TW_salad	REAL	*)	Transpired water per plant “v”	(kg)water / (m2s)

	TW_soybean TW_onion TW_spinach				

*) Values are listed in Figure 3-10 and Figure 3-11

A.3.7.3 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
$E_{lip\_1,v}$	C_lip_tomato1 H_lip_tomato1 O_lip_tomato1 N_lip_tomato1 S_lip_tomato1 P_lip_tomato1 Analogue for Potato Wheat Rice Salad Soybean Onion Spinach	REAL	CHONSP composition of lipids in biomass of given plant species	-
$E_{m\_HPc,v}$	C_prot[Crops] C_lip[Crops] C_ch[Crops], C_fib[Crops] C_RNA[Crops] C_DNA[Crops] C_HPre[Crops] Analogue for H O N S P	REAL	Relative CHONSP composition of macromolecules "m_HPc" of each plant species	-
CY_v	CY[Crops]		Crop Yield	kg/(m^{2}s)
$(f_{H2O,com})_v$	f_H2O_c[Crops]		Mass fraction of water in damp edible part of higher plant's "v" biomass	-
$(f_{H2O,re})_v$	f_H2O_re[Crops]		Mass fraction of water in damp residual biomass of higher plants "v"	-
$(f_{m\_HPc,com})_v$	f_prot[Crops] f_lip[Crops] f_ch[Crops] f_fib[Crops] f_arn[Crops] f_adn[Crops]	REAL	Mass fraction of macromolecules "m_HPc" on the dry mass of comestible higher plants "v"	-
$(f_{re,com})_v$	f_re[Crops]	REAL	Mass fraction of the residual part of the plant within the edible part of the plant "v" in kilograms of waste per kg of edible plant "v" (dry weight)	-
$M_{lipsat,v}$ $M_{lipinsat,v}$	M_lip_sat_tomato M_lip_insat_tomato Analogue for Potato Wheat Rice Salad Soybean Onion Spinach	REAL	Molecular weight of lipids of each plant species	kg/mol

$M_{m\_HPC,v}$	`M_prot[Crops]`
	`M_lip[Crops]`
	`M_ch[Crops]`
	`M_fib[Crops]`
	`M_adn[Crops]`
	`M_arn[Crops]`
	`M_HPre[Crops]`
	`M_HPc[Crops]`
	`M_plant[Crops]`
		REAL	Molecular weight of macromolecules “m_HPC” of the different plant species	kg/mol

TW_v	`TW[Crops]`	REAL	Transpired water of each plant “v”	kg/(m^2s)

A.3.7.4 Formulation

Details on mathematical model see chapter 3.7.1

A.3.8 Food Treatment Unit

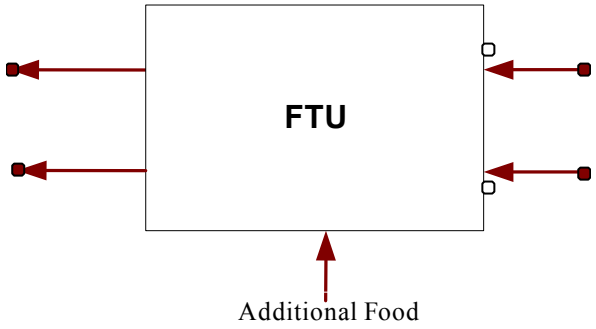
A.3.8.1 Description

This component type, named `Food_Treatment_Unit`, represents the process that participates in preparing food for the crew. It receives inflows of biomass from the high plant chamber and from Compartment IVa. Furthermore it receives a certain quantity of biomass from outside the MELiSSA loop that offers the nutrients and the vitamins that the food from the loop cannot offer. As outflows there are eatable and non-eatable parts of plants. The first are send to the crew compartments and the latter for recycling to the Biomass Pre-treatment Unit (BPU) and then to compartment I.

The purpose of the mathematic model of this unit is to determine the additional biomass composition that must to be supplied from outside the loop. Therefore, an equilibrate diet for one person must be defined as baseline data.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.8.2 Symbol



Food_Treatment_Unit

A.3.8.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`plant_in`	Plants		IN	Inflow of higher plants
`solid_Ap`	Solids	(mix=Compounds)	IN	Inflow of Arthrospira platensis
`sensor_Ap`	Sensor		IN	Sensor for the edible organic matter of Arthrospira platensis
`sensor_HPc`	Sensor		IN	Sensor for the edible organic matter of higher plants
`food_out`	Food		OUT	Outflow of food
`plant_out`	Solids	(mix=Compounds)	OUT	Outflow of non-eatable parts of higher plants

A.3.8.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS

$E_{m,food}$	`C_prot_food`
	`H_prot_food`
	`O_prot_food`
	`N_prot_food`
	`S_prot_food`
	`P_prot_food`
	
	`C_lip_food`
	`H_lip_food`
	`O_lip_food`
	`N_lip_food`
		REAL	1
			1.526
			0.327
			0.2496
			0.016
			0
			
			1
			1.714
				Relative CHONSP composition of the macromolecules "m" of the food (in dry weight)	-

	S_lip_food P_lip_food C_ch_food H_ch_food O_ch_food N_ch_food S_ch_food P_ch_food		0.204 0 0 0.020 1 1.67 0.711 0 0 0		
$f_{H2O,\ food}$	f_H2O_food	REAL	0.9	Mass fraction of water on the damp food	-
$f_{m,\ food}$	f_prot_food f_lip_food f_ch_food	REAL	0.2125 0.1497 0.6379	Mass fraction of each macromolecule on the dry food	-
n	n_crew	REAL	4	Number of crew members	-
$W_{food,\ indiv}$	W_food_1_person	REAL	$1.85e^{-5}$	Mass flow of food for one person (in dry weight)	kg/s

A.3.8.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
E_{adF_1}	C_ad1 H_ad1 O_ad1 N_ad1 S_ad1 P_ad1	REAL	CHONSP composition of additional food (in dry weight)	-
E_{adF}	C_ad H_ad O_ad N_ad S_ad P_ad	REAL	Relative CHONSP composition of additional food (in dry weight)	-
E_{food}	C_food1 H_food1 O_food1 N_food1 S_food1 P_food1	REAL	CHONSP composition of food (in dry weight)	-
E_{m,adF_1}	C_prot_ad1 C_lip_ad1 C_ch_ad1 H_prot_ad1 H_lip_ad1 H_ch_ad1 O_prot_ad1 O_lip_ad1 O_ch_ad1 N_prot_ad1 N_lip_ad1 N_ch_ad1 S_prot_ad1 S_lip_ad1 S_ch_ad1 P_prot_ad1 P_lip_ad1 P_ch_ad1	REAL	CHONSP composition of the macromolecules of additional food (in dry weight)	-
$E_{m,adF}$	C_prot_ad C_lip_ad C_ch_ad H_prot_ad H_lip_ad	REAL	Relative CHONSP composition of the macromolecules of additional food (in dry weight)	-

	H_ch_ad O_prot_ad O_lip_ad O_ch_ad N_prot_ad N_lip_ad N_ch_ad S_prot_ad S_lip_ad S_ch_ad P_prot_ad P_lip_ad P_ch_ad			
$f_{m,adF}$	f_prot_adF f_ch_adF f_lip_adF		Mass fraction of each macromolecule of additional food in the dry additional food	-
$f_{H2O,adF}$	f_H2O_adF		Mass fraction of water in the damp additional food	
M_{adF}	M_adF	REAL	Molecular weight of additional food	kg/mol
$M_{m,food}$	M_prot_food M_lip_food M_ch_food	REAL	Molecular weight of each macromolecule of food	kg/mol
W_{adF}	W_adF	REAL	Mass flow of additional food	kg/s
$W_{m,a}$	W_prot[Food_compounds] W_lip[Food_compounds] W_ch[Food_compounds]		Mass flow of each macromolecule of each food compounds (Arthrospira, Higher plants, additional food)	kg/s
$W_{m,food}$	W_prot_food W_lip_food W_ch_food	REAL	Mass flow of each macromolecule of food	kg/s
$W_{H2O,adF}$	W_H2O_adF	REAL	Mass flow of water contained in additional food	kg/s
$W_{H2O,food}$	W_H2O_food	REAL	Mass flow of water contained in food	kg/s
$W_{H2O,HPre}$	W_H2O_HPre	REAL	Mass flow of water contained in residue of higher plants	kg/s
$Z_{a,in}$	Z_in[Food_components]	REAL	Inlet molar flow of each food compounds	mol/s
Z_{food}	Z_food	REAL	Molar flow of food	mol/s

A.3.8.6 Formulation

Details on mathematical model see chapter 3.8.1

A.3.9 Liquid Collector and Distributor

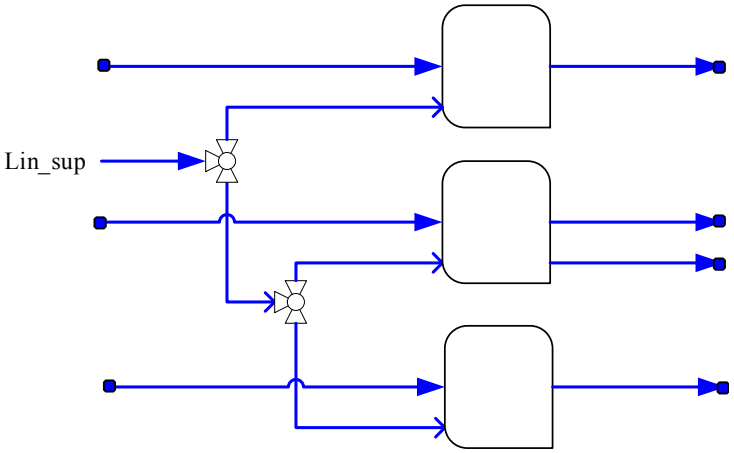
A.3.9.1 Description

This component type, named `Liquid_Collector_Distributor`, represents the process of collecting and distributing liquids. The liquid inflows are of potable water and hygiene water. The liquid outflows are potable and hygiene water for mainly the Crew, the Artrospira Washing and BPU.

The mathematic model calculates the quantity of additional water (water supply) required.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.9.2 Symbol



Liquid_Collector_Distributor

A.3.9.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in_hyg`	Liquid	(mix=Water)	IN	Inflow of hygiene water
`liq_in_loop`	Liquid		IN	Inflow of liquid from the loop
`liq_in_pot`	Liquid	(mix=Water)	IN	Inflow of potable water
`liq_out_Ap`	Liquid	(mix=Compounds)	OUT	Outflow of hygiene water for the Arthrospira Washing
`liq_out_CI`	Liquid	(mix=Compounds)	OUT	Outflow of Liquid for the CI
`liq_out_hyg_crew`	Liquid	(mix=Water)	OUT	Outflow of hygiene water for the crew
`liq_out_pot_crew`	Liquid	(mix=Water)	OUT	Outflow of potable water for the crew

A.3.9.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
n	`n_crew`	REAL	4	Number of crew members	-
$Q^{indiv}_{hyg,CC}$	`Q_hyg_crew`	REAL	1.65 e^{-7}	Volumetric flow of hygiene water required per person	m^3/s
$Q_{L,CI}$	`Q_liq_CI`	REAL	5 e^{-7}	Volumetric flow of water required for CI	m^3/s
$Q^{indiv}_{pot,CC}$	`Q_pot_crew`	REAL	3 e^{-8}	Volumetric flow of drinking water required per person	m^3/s
$Q_{hyg,WA}$	`Q_water_Ap`	REAL	1.75e^{-8}	Volumetric flow of water required for AW	m^3/s

A.3.9.5 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS

$Q_{H2O\_CI,ad}$	Q_ad_CI	REAL	Additional volumetric flow of water to fulfil the requirements of CI	m^3/s
$Q_{hyg,ad}$	Q_ad_hyg	REAL	Additional volumetric flow of hygiene water to fulfil the requirements of the crew and of the AW	m^3/s
$Q_{pot,ad}$	Q_ad_pot	REAL	Additional volumetric flow of potable water to fulfil the requirements of the crew	m^3/s
Q_{Lin_sup}	Q_sup	REAL	Total additional volumetric flow of water to supply	m^3/s

A.3.9.6 Formulation

Details on mathematical model see chapter 3.8.2

A.3.10 Biomass Pre-treatment Unit

A.3.10.1 Description

This component type, named `Biomass_Pretreatment_Unit`, represents a biomass pre-treatment unit. The biomass of *R. Rubrum* from CII, *Nitrosomas* and *Nitrobacter* from CIII, residual higher plants from the Food Treatment Unit (FTU) and faeces from the Crew Compartment are all collected in the BPU, mixed with water usually coming from the Liquid Separator and Distributor (LSD). In the BPU the biomass is pre-treated physico-chemically to speed up the anaerobic degradation of the biomass-water suspension that is send via the liquid outflow to Compartment I.

The mathematic model applied for the BPU is only representing mathematically the biomasses mix, which is expressed as only one mass called Residual Biomass (RB) containing a CHONSP composition resulted from the mix:

$$[\mathrm{CHONSP}]_{\mathrm{R.\,rubrum}} + [\mathrm{CHONSP}]_{\mathrm{Nitrosomonas\ -\ Nitrobacter}} + [\mathrm{CHONSP}]_{\mathrm{HPS\,residual}} + [\mathrm{CHONSP}]_{\mathrm{faeces}}$$

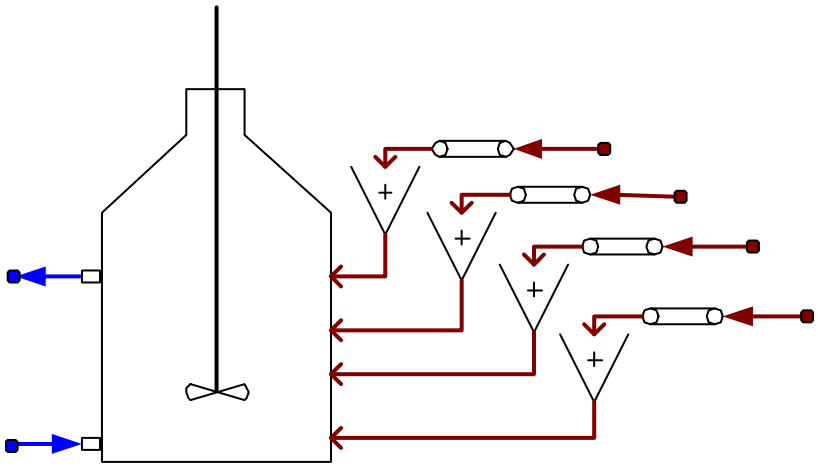
$$\Downarrow$$

$$[\mathrm{CHONSP}]_{\mathrm{Residual\,Biomass}}$$

Thus, the mathematic model objective is to determine the volumetric flow of the outlet stream and its composition.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc.

A.3.10.2 Symbol



Biomass_Pretreatment_Unit

A.3.10.3 Ports

NAME	TYPE	DIRECTION	DESCRIPTION
`liq_in`	Liquid	IN	Liquid inflow
`liq_out`	Liquid	OUT	Liquid outflow
`solid_Fc`	Solid	IN	Solid inflow of faeces
`solid_HPre`	Solid	IN	Solid inflow of higher plant's residue
`solid_New`	Solid	IN	Solid inflow of Nitrosomas and Nitrobacter
`solid_Rr`	Solid	IN	Solid inflow of R. Rubrum

A.3.10.4 Variables

NAME	SYMBOL	TYPE	DESCRIPTION	UNITS
E_b	C_bio[Biomass_NC] H_bio[Biomass_NC] O_bio[Biomass_NC] N_bio[Biomass_NC] S_bio[Biomass_NC] P_bio[Biomass_NC]	REAL	Relative CHONSP composition of each biomass (non-comestible biomass) form the residual biomass (in dry weight)	-
E_{RB}	C_RB H_RB O_RB N_RB S_RB P_RB	REAL	Relative CHONSP composition of the residual biomass (in dry weight)	-
E_{RB_1}	C_RB1 H_RB1 O_RB1 N_RB1 S_RB1 P_RB1	REAL	CHONSP composition of residual biomass (in dry weight)	-
$f_{H2O,RB}$	f_H2O_RB	REAL	Mass fraction of water in damp residual biomass	
$f_{m,RB}$	f_prot_RB f_lip_RB f_ch_RB	REAL	Mass fraction of each macromolecule in dry residual biomass	-
M_{RB}	M_RB	REAL	Molecular weight of residual biomass	kg/mol
$W_{H2O,b}$	W_H2O_Rr W_H2O_New W_H2O_Fc W_H2O_HPre	REAL	Mass flow of water contained in each biomass form the residual biomass	kg/s
$W_{H2O,RB}$	W_H2O_RB		Mass flow of water contained in residual biomass	kg/s
$W_{RB,Lout}$	W_dry_RB	REAL	Mass flow of dry residual biomass	kg/s
$Z_{i,in}$	Z_in[Compounds]	REAL	Molar inflow of each compound	mol/s

A.3.10.5 Formulation

Details on mathematical model see chapter 3.8.3

A.3.11 Solid-Liquid Separator

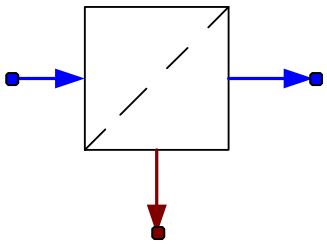
A.3.11.1 Description

This component type, named `Solid_Liquid_Separator`, represents the processes of solid-liquid separation, to precipitate the biomass particles form the liquid. It has one liquid inflow usually coming from a connected bioreactor and two outflows – one liquid and one solid. The separated biomass is sent to the Solid Distributor, while the liquid flows to the next compartment.

The objective is to obtain the new outlet concentrations and the volumetric flows in both the solid stream and the liquid stream.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.11.2 Symbol



Solid_Liquid_Separator

A.3.11.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid inflow
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid outflow
`solid_out`	Solid	(mix = Compounds)	OUT	Solid Outflow

A.3.11.4 Data

NAME	SYMBOL	DEFAULT	DESCRIPTION	UNITS
$f_{don,bio}$	`f_don_bio`	1000	Mass fraction of the dissolution that biomass retains; the kilograms of dissolution per kilogram of damp biomass	-
ρ_{don}	`d_don`	1000	Density of the dissolution	kg/m^3

A.3.11.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$c_{i,don}$	`Con_don[Compounds]`	REAL	Molar concentration of each compound in the dissolution	mol/m^3
$\frac{W_{bio,Lin}}{\rho_{bio}}$	`Q_bio_solid_out`	REAL	Volumetric flow of damp biomass at the solid outlet stream	m^3/s
$\frac{W_{bio,Lin} \cdot f_{don,bio}}{\rho_{don}}$	`Q_don_solid_out`	REAL	Volumetric outflow of dissolution at the solid outlet stream	m^3/s
$W_{damp\_bio,Lin}$	`W_bio[Biomass]`	REAL	Mass flow of each damp biomass at the liquid inflow	kg/s
$W_{damp\_bio,Lin}$	`W_bio_in`	REAL	Mass flow of the whole damp biomass at the liquid inflow	kg/s
$W_{don,Lin}$	`W_don_in`	REAL	Mass flow of the dissolution at the	kg/s

			liquid inflow	
$W_{i,Lin}$	`W_in[Compounds]`	REAL	Mass flow of each compound at the liquid inflow	kg/s
W_{Lin}	`W_liq_in`	REAL	Mass flow of liquid at the liquid inflow	kg/s
ρ_L	`d_liq_in`	REAL	Density of the liquid	kg/m^3
ρ_{bio}	`d_bio`	REAL	Density of damp biomass	kg/m^3

A.3.11.6 Formulation

Details on mathematical model see chapter 3.8.4

A.3.12 Atmosphere Generator

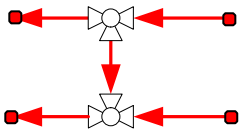
A.3.12.1 Description

This component type, named `Atmosphere_Generator`, represents the production of breathable atmosphere for the crew at the required pressure and temperature. One gas inflow is from the Molecular Oxygen Collector (MOC) the other for pure nitrogen that might be needed. The resulting outflow is a composition of gases optimal for humans and is usually send to the crew compartment and BR_CIII.

The objective of the mathematic model is to obtain the necessary molar flow of nitrogen to achieve the crew requirements.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.12.2 Symbol



Atmosphere_Generator

A.3.12.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
gas_in	Gas	(mix = Gas_Liquid)	IN	Gas Inflow
gas_in_sup	Gas	(mix = Gas_Liquid)	IN	Supply Inflow
gas_out	Gas	(mix = Gas_Liquid)	OUT	Gas Outflow
gas_out_sup	Gas	(mix = Gas_Liquid)	OUT	Supply Outflow

A.3.12.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
$H_{N2,O2}$	H_N2_O2	REAL	4	Molar relation between nitrogen and oxygen	-
Pr	Pr	REAL	$1.01325e^5$	Pressure outlet	Pa
T	T	REAL	298	Temperature outlet	K

A.3.12.5 Variables

NAME	SYMBOL	TYPE	Description	Units
Q_{ad}	Q_ad	REAL	Volumetric flow necessary to fulfil the requirements	m^3/s
R	R = 8.31434	CONST REAL	Ideal gas constant	(Pa m^3)/(mol K)
W_{N2,Gin_ad}	W_N2_ad	REAL	Mass flow of additional nitrogen	kg/s
$W_{i,in}$	W_in[Gas_Liquid]	REAL	Mass inflow of each compound	kg/s
$W_{i,out}$	W_out[Gas_Liquid]	REAL	Mass outflow of each compound	kg/s
$W_{total,in}$	W_total_in	REAL	Mass total inflow	kg/s
$W_{total,out}$	W_total_out	REAL	Mass total outflow	kg/s
$Z_{i,Gin}$	Z_in_gas[Gas_Liquid]	REAL	Molar inflow of each compound at the gas inlet stream	mol/s
Z_{i,Gin_sup}	Z_in_sup[Gas_Liquid]	REAL	Molar inflow of each compound at the supply inlet	mol/s

			stream	
$Z_{i,Gout}$	`Z_out_gas[Gas_Liquid]`	REAL	Molar outflow of each compound at the gas outlet stream	mol/s
$Z_{i,Gout\_sup}$	`Z_out_sup[Gas_Liquid]`	REAL	Molar outflow of each compound at the supply outlet stream	mol/s
$Z_{N2,ad}$	`Z_N2_ad`	REAL	Molar flow of additional nitrogen	mol/s

A.3.12.6 Formulation

Details on mathematical model see chapter 3.8.5

A.3.13 Gas Distributor

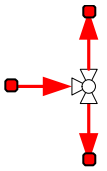
A.3.13.1 Description

This component type, named `Gas_Distributor`, represents a valve with the function to distribute the inflow. It has one gas inflow and two outflows.

For MELiSSA three Gas Distributors are considered.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.13.2 Symbol



Gas_Distributor

A.3.13.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
gas_in	Gas	(mix = Gas_Liquid)	IN	Gas Inflow
gas_out_A	Gas	(mix = Gas_Liquid)	OUT	Gas outflow stream A
gas_out_B	Gas	(mix = Gas_Liquid)	OUT	Gas outflow stream B

A.3.13.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
D_A	D_A	REAL	0.5	Flow rate between the ingoing and outgoing A stream	-

A.3.13.5 Formulation

Details on mathematical model see chapter 3.8.6

A.3.14 Liquid Distributor

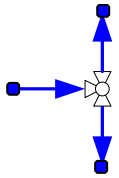
A.3.14.1 Description

This component type, named `Liquid_Distributor`, represents a valve with the function to distribute the inflow. It has one liquid inflow and two outflows.

For MELiSSA one Liquid Distributor has been considered, which receives the filtered liquid from the nitrifying bioreactor in order to distribute it between the two photosynthetic compartments.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.14.2 Symbol



Liquid_Distributor

A.3.14.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid Inflow
`liq_out_A`	Liquid	(mix = Compounds)	OUT	Liquid outflow stream A
`liq_out_B`	Liquid	(mix = Compounds)	OUT	Liquid outflow stream B

A.3.14.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
D_A	`D_A`	REAL	0.5	Flow rate between the ingoing and outgoing A stream	-

A.3.14.5 Formulation

Details on mathematical model see chapter 3.8.6

A.3.15 Solid Distributor

A.3.15.1 Description

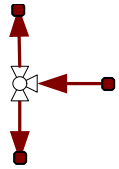
This component type, named `Solid_Distributor`, represents a valve with the function to distribute the inflow. It has one solid inflow and two outflows.

For MELiSSA five solid distributors are considered; one for each biomass:

- *Arthrospira*
- *R. rubrum*,
- *Nitrosomonas* and *Nitrobacter*,
- Non-eatable parts of higher plants
- faeces

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.15.2 Symbol



Solid_Distributor

A.3.15.3 Ports

NAME	TYPE	DIRECTION	DESCRIPTION
`solid_in`	Solid	IN	Solid inflow
`solid_out_A`	Solid	OUT	Solid outflow stream A
`solid_out_B`	Solid	OUT	Solid outflow stream B

A.3.15.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
D_A	`D_A`	REAL	0.5	Flow rate between the ingoing and outgoing A stream	-

A.3.15.5 Formulation

Details on mathematical model see chapter 3.8.6

A.3.16 Gas Collector

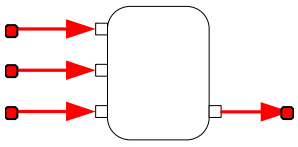
A.3.16.1 Description

This component type, named `Gas_Collector`, represents the collection of different gas streams to merge them into one.

Through the mathematic model the concentration of each compound and the volumetric flow of the resulting stream is obtained.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.16.2 Symbol



Gas_Collector

A.3.16.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in_1`	Gas	(mix = Gas_Liquid)	IN	Gas inflow stream 1
`gas_in_2`	Gas	(mix = Gas_Liquid)	IN	Gas inflow stream 2
`gas_in_3`	Gas	(mix = Gas_Liquid)	IN	Gas inflow stream 3
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas outflow

A.3.16.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
Pr	`Pr`	REAL	$1.01325e^{5}$	Pressure of the outlet gas	Pa
T	`T`	REAL	298	Temperature of the outlet gas	K

A.3.16.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$Z_{i,Ein\ A}$	`Z_in_1[Compounds]`	REAL	Molar inflow of each compound at stream 1	mol/s
$Z_{i,Ein\ B}$	`Z_in_2[Compounds]`	REAL	Molar inflow of each compound at stream 2	mol/s
$Z_{i,Ein\ C}$	`Z_in_3[Compounds]`	REAL	Molar inflow of each compound at stream 3	mol/s
Z_{Eout}	`Z_out[Compounds]`	REAL	Molar outflow of each compound	mol/s

A.3.16.6 Formulation

Details on mathematical model see chapter 3.8.7

A.3.17 Liquid Collector

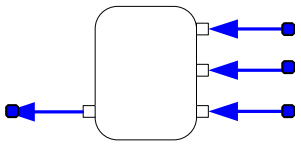
A.3.17.1 Description

This component type, named `Liquid_Collector`, represents the collection of different liquid streams to merge them into one.

In the applied mathematic model the concentration of each compound and the volumetric flow of the resulting stream is obtained.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.17.2 Symbol



Liquid_Collector

A.3.17.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in_1`	Liquid	(mix = Compounds)	IN	Liquid inflow of stream 1
`liq_in_2`	Liquid	(mix = Compounds)	IN	Liquid inflow of stream 2
`liq_in_3`	Liquid	(mix = Compounds)	IN	Liquid inflow of stream 3
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid outflow

A.3.17.4 Variables

NAME	SYMBOL	TYPE	Description	Units
$Z_{i,Ein\ A}$	`Z_in_1[Compounds]`	REAL	Molar inflow of each compound at stream 1	mol/s
$Z_{i,Ein\ B}$	`Z_in_2[Compounds]`	REAL	Molar inflow of each compound at stream 2	mol/s
$Z_{i,Ein\ C}$	`Z_in_3[Compounds]`	REAL	Molar inflow of each compound at stream 3	mol/s
Z_{Eout}	`Z_out[Compounds]`	REAL	Molar outflow of each compound	mol/s

A.3.17.5 Formulation

Details on mathematical model see chapter 3.8.7

A.3.18 Condenser

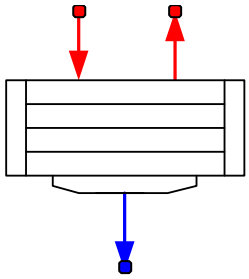
A.3.18.1 Description

This component type, named `Condenser`, represents the condensation of water in the gas e.g. the water transpired by the higher plants.

Through the mathematic model the concentration of each compound in the resulting gas, the volumetric outflow and the quantity of condensed water is described.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.18.2 Symbol



Condenser

A.3.18.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
gas_in	Gas	(mix = Gas_Liquid)	IN	Gas Inflow
gas_out	Gas	(mix = Gas_Liquid)	OUT	Gas Outflow
liq_out	Liquid	(mix = Water)	OUT	Liquid Outflow

A.3.18.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
Pr	Pr	REAL	$1.0132e^5$	Pressure	Pa
T	T	REAL	298	Bioreactor Temperature	K

A.3.18.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$h_{H2O,Gin}$	h1_H2O	REAL	Molar fraction of water in the gas	-
$h_{H20,sat}$	h2_H2O	REAL	Molar fraction of water in saturation conditions	-
$H_{H2O,Gin}$	H1_H2O	REAL	Molar ratio of water in gas; mols of water per mols of rest	-
$H_{H2O,sat}$	H2_H2O	REAL	Molar ratio of water in saturation conditions; mols of water per mols of rest in saturation conditions	-
$P_{sat,\ H20}$	p_H2O	REAL	Partial pressure of water	Pa
R	R = 8.31434	CONST REAL	Ideal gas constant	(Pa m^3)/(mol K)
TC	TC	REAL	Temperature in centigrade	ºC
$Z_{i,Gin}$	Z_in[Gas_Liquid]	REAL	Molar inflow of each compounds	mol/s

Z_{Gin}	Z_total	REAL	Total molar inflow	mol/s
$(Z_{Gin} - Z_{H2O,Gin})$	Z_rest	REAL	Total molar flow without considering water	mol/s
$Z_{H2O,cond}$	Z_liq_H2O	REAL	Molar flow of condensated water	mol/s
$Z_{i,Gout}$	Z_gas_out[Gas_Liquid]	REAL	Molar flow at the gas outlet	mol/s

A.3.18.6 Asserts

```
ASSERT ((TC> - 273.15 AND TC < 374.15)) WARNING \
            "Temperature out of range in H2O_psat Function"
```

A.3.18.7 Formulation

Details on mathematical model see chapter 3.8.8

A.3.19 Arthrospira Washing

A.3.19.1 Description

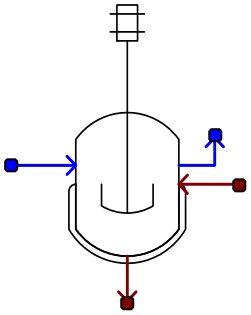
This component type, named `Arthrospira_Washing`, represents the *A. platensis* washing with the aim to eliminate the solute (ammonia, nitrates, sulphates, phosphates, carbonates, etc.) that accompanies this biomass.

The mathematic model is applicable to eache stage in the washing process, whichis represented by a stirred tank where the algae are partially cleaned.

The objective of the equations is to obtain the volumetric flows and the concentrations in the outlet streams of the AW.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.19.2 Symbol



Arthrospira_Washing

A.3.19.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid Inflow
`liq_out`	Liquid	(mix = Compounds)	OUT	Liquid Outflow
`solid_in`	Solid	(mix = Compounds)	IN	Solid Inflow
`solid_out`	Solid	(mix = Compounds)	OUT	Solid Outflow

A.3.19.4 Data

NAME	Symbol	TYPE	DEFAULT	DESCRIPTION	UNITS
ρ_{don}	`d_don`	REAL	`1000`	Density of the dissolution. It is the density of the liquid without considering the biomass	kg/m^3

A.3.19.5 Variables

NAME	SYMBOL	TYPE	Description	Units
C_{don}	`Con_don[Compounds]`	REAL	Molar concentration of each compound at the dissolution	mol/m^3
$C_{solute.Lin'}$	`Con_solut_liq_in`	REAL	Molar concentration of the solute at the liquid inlet	mol/m^3
$C_{solute,Lout'}$	`Con_solut_liq_out`	REAL	Molar concentration of the solute at the liquid outlet	mol/m^3
$C_{solute,don,Sin'}$	`Con_solut_solid_in`	REAL	Molar concentration of the solute at the solid inlet	mol/m^3
$C_{solute,don,Sout'}$	`Con_solut_solid_out`	REAL	Molar concentration of the solute at the solid outlet	mol/m^3
$Q_{don,Sin'}$	`Q_don_solid_in`	REAL	Volumetric flow of dissolution at the solid inlet	m^3/s

$W_{damp\_bio,Sin'}$	W_bio_solid_in	REAL	Mass flow of biomass at the solid inlet	kg/s
$W_{don.Sin'}$	W_don_solid_in	REAL	Mass flow of dissolution at the solid inlet	kg/s
$W_{i,Sin'}$	W_solid_in[Compounds]	REAL	Mass flow of each compound at the solid inlet	kg/s
$W_{Sin'}$	W_total_solid_in	REAL	Mass total flow at the solid inlet	kg/s
h_i	h_don[Compounds]	REAL	Molar fraction of each compound at the dissolution	-
$Z_{i,Sin'}$	Z_solid_in[Compounds]	REAL	Molar flow of each compound at the solid inlet	mol/s
$Z_{solute,Sin'}$	Z_solut_solid_in	REAL	Molar flow of solute at the solid inlet	mol/s
r_{bio}	d_bio	REAL	Density of biomass	kg/m^3
r_{Sin}	d_solid_in	REAL	Density of the solid inlet	kg/m^3

A.3.19.6 Formulation

Details on mathematical model see chapter3.8.9

A.3.20 Purge - Gas

A.3.20.1 Description

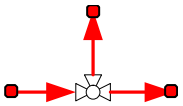
This component type, named `Purge_Gas`, represents the removal of certain products from the gas system to avoid accumulation.

Physically a purge can be exactly like a valve and mathematically behaves as a Distributor.

The objective of the mathematic model is to calculate the volumetric outflows.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.20.2 Symbol



Purge_Gas

A.3.20.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
gas_in	Gas	(mix = Gas_Liquid)	IN	Gas Inflow
gas_out	Gas	(mix = Gas_Liquid)	OUT	Recycled Gas Outflow
gas_out_P	Gas	(mix = Gas_Liquid)	OUT	Purged (removed) Gas Outflow

A.3.20.4 Variables

NAME	SYMBOL	TYPE	Description	Units
r	r	REAL	Coefficient that relates the recycled volumetric outflow with the inflow	-

A.3.20.5 Formulation

Details on mathematical model see chapter 3.8.10

A.3.21 Purge – Liquid

A.3.21.1 Description

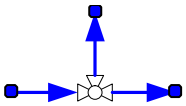
This component type, named `Purge_Liquid`, represents the removal of certain products from the liquid system to avoid accumulation.

Physically a purge can be exactly like a valve and mathematically behaves as a Distributor.

The objective of the mathematic model is to calculate the volumetric outflows.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.21.2 Symbol



Purge_Liquid

A.3.21.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in`	Liquid	(mix = Compounds)	IN	Liquid Inflow
`liq_out`	Liquid	(mix = Compounds)	OUT	Recycled Liquid Outflow
`liq_out_P`	Liquid	(mix = Compounds)	OUT	Purged (removed) Liquid Outflow

A.3.21.4 Variables

NAME	SYMBOL	TYPE	Description	Units
r	`r`	REAL	Coefficient that relates the recycled volumetric outflow with the inflow	-

A.3.21.5 Formulation

Details on mathematical model see chapter 3.8.10

A.3.22 Union Point - Liquid

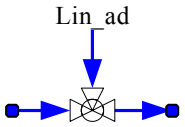
A.3.22.1 Description

This component type, named `Union_Point_Liquid`, represents the merging of the liquid flows from within the system and additional substance needed from outside.

The mathematic model objective is to obtain the additional flow, as well as the outflow of the Union Point. The added compounds are substances dissolved in water with a known concentration.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.22.2 Symbol



Union_Point_Liquid

A.3.22.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
liq_in	Liquid	(mix = Compounds)	IN	Liquid Inflow
liq_out	Liquid	(mix = Compounds)	OUT	Liquid Outflow

A.3.22.4 Data

NAME	TYPE	DEFAULT	DESCRIPTION	UNITS
Con_Ac	REAL	0	Molar concentration of Ac	mol/m^3
Con_Ap	REAL	o	Molar concentration of A. platensis	mol/m^3
Con_But	REAL	0	Molar concentration of But	mol/m^3
Con_Cap	REAL	0	Molar concentration of Cap	mol/m^3
Con_CH4	REAL	0	Molar concentration of Methane	mol/m^3
Con_CO2	REAL	0	Molar concentration of CO2	mol/m^3
Con_Fc	REAL	0	Molar concentration of Faeces Biomass	mol/m^3
Con_HNO3	REAL	0	Molar concentration of HNO3	mol/m^3
Con_HPc	REAL	0	Molar concentration of eatable biomass of higher plants	mol/m^3
Con_HPre	REAL	0	Molar concentration of High Plants non-comestible Biomass	mol/m^3
Con_H2	REAL	0	Molar concentration of H2	mol/m^3
Con_H2O	REAL	5555,56	Molar concentration of H2O	mol/m^3
Con_H3PO4	REAL	0	Molar concentration of H3PO4	mol/m^3
Con_H2SO4	REAL	0	Molar concentration of H2SO4	mol/m^3
Con_New	REAL	0	Molar concentration of Nitrosomonas and Nitrobacter Biomass	mol/m^3
Con_NH3	REAL	0	Molar concentration of NH3	mol/m^3
Con_N2	REAL	0	Molar concentration of N2	mol/m^3
Con_O2	REAL	0	Molar concentration of O2	mol/m^3
Con_Prop	REAL	0	Molar concentration of Prop	mol/m^3
Con_RB	REAL	0	Molar concentration of Residual Biomass	mol/m^3
Con_Rr	REAL	0	Molar concentration of Rodhobacter Biomass	mol/m^3
Con_Val	REAL	0	Molar concentration of Val	mol/m^3

A.3.22.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$c_{i,ad}$	Con_ad[Compounds]	REAL	Molar concentration of each compound at the additional stream	mol/m^3
Q_{Ein_ad}	Q_in_ad	REAL	Additional volumetric flow added	m^3/s
Z_{i,Ein_ad}	Z_ad[Compounds]	REAL	Additional molar flow of each compound	mol/s
$Z_{i,Eout}$	Z_out[Compounds]	REAL	Molar outflow of each compound	mol/s

A.3.22.6 Formulation

Details on mathematical model see chapter 3.8.11

A.3.23 Union Point - Gas

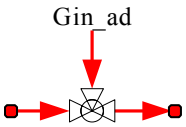
A.3.23.1 Description

This component type, named `Union_Point_Gas`, represents the merging of the gas flows from within the system and additional substance needed from outside.

The mathematic model objective is to obtain the additional flow, as well as the outflow of the Union Point. The additional gas stream contains pure compounds.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.23.2 Symbol



Union_Point_Gas

A.3.23.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in`	Gas	(mix = Gas_Liquid)	IN	Gas Inflow
`gas_out`	Gas	(mix = Gas_Liquid)	OUT	Gas Outflow

A.3.23.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
Pr	`Pr`	REAL	$1.01325e^{5}$	Pressure	Pa
T	`T`	REAL	298	Temperature	K

A.3.23.5 Variables

NAME	SYMBOL	TYPE	Description	Units
R	`R = 8.31434`	CONST REAL	Ideal gas constant	(Pa m^3) / (mol K)
$Z_{i,ad}$	`Z_ad[Compounds]`	REAL	Additional molar flow of each compound	mol/s
$Z_{i,out}$	`Z_out[Compounds]`	REAL	Molar outflow of each compound	mol/s

A.3.23.6 Formulation

Details on mathematical model see chapter 3.8.11

A.3.24 Evaporator

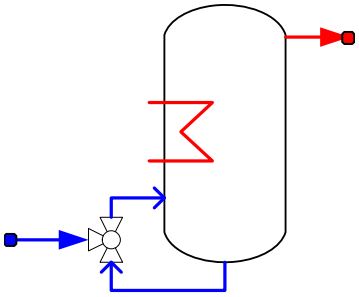
A.3.24.1 Description

This component type, named `Evaporator`, represents water production, which is utilized at controlled temperature during the CO_2 desorption process. The required thermal energy is supplied by electrical current.

Through the mathematic model the evaporation temperature is calculated.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.24.2 Symbol



Evaporator

A.3.24.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`water_in`	Water	(mix = Water)	IN	Water inflow
`steam_out`	Gas	(mix = Water)	OUT	Steam outflow

A.3.24.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
Pr	`Pr`	REAL	$1.01325e^5$	Pressure at the gas outlet	Pa

A.3.24.5 Variables

NAME	SYMBOL	TYPE	Description	Units
R	`R = 8.31434`	CONST REAL	Ideal gas constant	(Pa m^3) / (mol K)
T	`T`	REAL	Temperature for evaporating	K
TC	`TC`	REAL	Temperature for evaporating	°C
$Z_{H2O,Lin}$	`Z_in_H2O`	REAL	Molar inflow of water	mol/s
$Z_{H2O,Gout}$	`Z_out_H2O`	REAL	Molar outflow of water	mol/s

A.3.24.6 Formulation

Details on mathematical model see chapter 4.4.1

A.3.25 Adsorber-Desorber

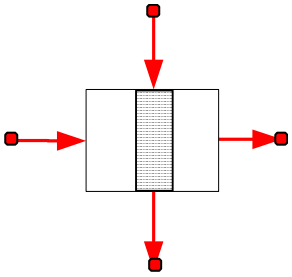
A.3.25.1 Description

This component type, named `Adsorber_Desorber`, represents the processes that separate the carbon dioxide from the air. Thus, it can represent several solid amine adsorber beds in which three main operation modes occur: adsorption, desorption and stand-by.

The objective of the mathematic model is to calculate the volumetric flows and the concentrations at the outlet of the system.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.25.2 Symbol



Adsorber_Desorber

A.3.25.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
gas_in_air	Gas	(mix = Gas_Liquid)	IN	Air inflow
gas_in_steam	Gas	(mix = Water)	IN	Steam inflow
gas_out_air	Gas	(mix = Gas_Liquid)	OUT	Air outflow
gas_out_CO2	Gas	(mix = Gas_Liquid)	OUT	CO_2 gas outflow

A.3.25.4 Data

NAME	Symbol	TYPE	DEFAULT	DESCRIPTION	UNITS
$H_{CO2,Am}$	H_CO2_Am	REAL	0.0591	Molar fraction of CO_2 adsorbed per mol of CO_2 that enters and per kg of amine	kg^{-1}
n_{bed}	n_bed	REAL	2	Numbers of beds	-
Pr	Pr	REAL	$1.01325e^5$	Average pressure at the outlets of the Adsorber-Desorber	Pa
T	T	REAL	298	Average temperature at the outlets of the Adsorber-Desorber	K
WS_{Am}	Ws_Am	REAL	7	Amine Mass in one bed	kg

A.3.25.5 Variables

NAME	SYMBOL	TYPE	Description	Units
R	R = 8.31434	CONST REAL	Ideal gas constant	(Pa m^3) / (mol K)
Z_{i,in_steam}	Z_in_steam[Water]	REAL	Molar flow of water at the steam inlet	mol/s
Z_{i,in_air}	Z_in_air[Gas_Liquid]	REAL	Molar flow of each compound at the gas inlet	mol/s
Z_{CO2_ads}	Z_CO2_ads	REAL	Molar flow of CO2 adsorbed (mol/s)	mol/s
$Z_{H2O,free}$	Z_H2O_free	REAL	Molar flow of H2O released	mol/s

			during the adsorption	
$Z_{i,Gout\_air}$	`Z_out_air[Gas_Liquid]`	REAL	Molar outflow of each compound at the air output	mol/s
$Z_{i,Gout\_CO2}$	`Z_out_CO2[Gas_Liquid]`	REAL	Molar outflow of each compound at the CO_2 gas output	mol/s
$W_{i,in}$	`W_in[Gas_Liquid]`	REAL	Mass inflow of each compound	kg/s
$W_{i,out}$	`W_out[Gas_Liquid]`	REAL	Mass outflow of each compound	kg/s
$W_{in,total}$	`W_total_in`	REAL	Total mass inflow	kg/s
$W_{out,total}$	`W_total_out`	REAL	Total mass outflow	kg/s

A.3.25.6 Formulation

Details on mathematical model see chapter 4.4.2

A.3.26 Sabatier Reactor

A.3.26.1 Description

This component type, named `Sabatier_Reactor`, represents the conversion of carbon dioxide and hydrogen to methane and water vapour. The stoichiometric relationship describing Sabatier CO_2 reduction process is given by:

$$CO_2 + 4\,H_2 \Leftrightarrow CH_4 + 2\,H_2O$$

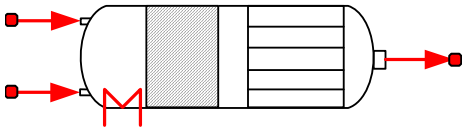
This reaction is exothermic and occurs in presence of a catalyst (ruthernium on alumina). The process takes place in two consecutive stages; the first under adiabatic conditions and the second under isothermal conditions. Therefore, the first stage takes place in an adiabatic cylindrical reactor tube, while the second one is in an air-cooled reactor.

The system model represents two Sabatier reactors connected in series. For the calculations the temperature is based on the second reactors', because at this temperature the thermodinamic equilibrium has been reached

The objective of the calculations is to obtain the volumetric flow and the concentrations of each compound at the reactor outlet.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.26.2 Symbol



Sabatier_Reactor

A.3.26.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`gas_in_A`	Gas	(mix = Gas_Liquid)	IN	Gas inflow of stream A
`gas_in_B`	Gas	(mix = Gas_Liquid)	IN	Gas inflow of stream B
`gas_out`	Gas	(mix = Gas_Liquid)	Out	Gas outflow

A.3.26.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
Pr	`Pr`	REAL	$1e^5$	Pressure outlet	Pa
T	`T`	REAL	523	Temperature outlet	K

A.3.26.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$G_{i,26}$	`G_26[Gas_Liquid]`	REAL	Generation of each compound due to the oxygen reduction	mol/s
$G_{i,27}$	`G_27[Gas_Liquid]`	REAL	Generation of each compound due to the carbon dioxide reduction	mol/s
$h_{i,out}$	`h_out[Gas_Liquid]`	REAL	Molar fraction of compounds in outflow	-
Kh	`Kh`	REAL	Molar equilibrium constant	-
Kp	`Kp`	REAL	Pressure Equilibrium constant	Atm^{-2}
R	`R = 8.31434`	CONST REAL	Ideal gas constant	(Pa m^3) / (mol

				K)
X_{H2}	X_H2	ALG REAL	Equilibrium conversion of Hydrogen	-
$Y_{i,26}$	Y_26[Gas_Liquid]	REAL	Stoichiometric coefficient of each compound in the oxygen reduction	-
$Y_{i,27}$	Y_27[Gas_Liquid]	REAL	Stoichiometric coefficient of each compound in the carbon dioxide reduction	-
$W_{i,in}$	W_in[Gas_Liquid]	REAL	Mass inflow of each compound	kg/s
$W_{i,out}$	W_out[Gas_Liquid]	REAL	Mass outflow of each compound	kg/s
$W_{total,in}$	W_total_in	REAL	Mass total inlfow	kg/s
$W_{total,out}$	W_total_out	REAL	Mass total outlfow	kg/s
$Z_{i,in}$	Z_in[Gas_Liquid]	REAL	Molar flow of each compound	mol/s
$Z_{i,out}$	Z_out[Gas_Liquid]	REAL	Molar flow of each compound	mol/s
$Z_{total,out}$	Z_total_out	REAL	Total molar outflow	mol/s

A.3.26.6 Formulation

Details on mathematical model see chapter 4.5.1

A.3.27 Electrolyser Stack

A.3.27.1 Description

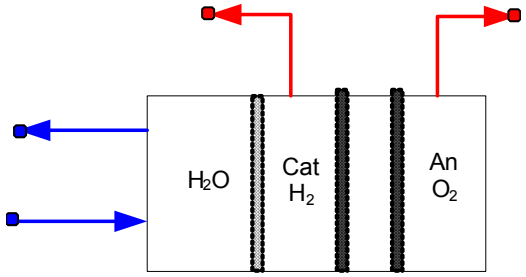
This component type, named `Electrolyser_Stack`, represents a method of separating chemically bonded elements and compounds by passing an electric current through them.

Thus, water enters to the electrolyser and is oxidized into oxygen that will appear at the anode (the positively charged electrode) and reduced into hydrogen that will appear at the cathode (the negatively charged electrode, where electrons are pumped into the water).

The electrolyser is subdivided in four adjacent compartments: feed water, cathode, electrolyte and anode.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.27.2 Symbol



Electrolyser

A.3.27.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
water_in	Water	(mix = Water)	IN	Water inflow
gas_out_An	Gas	(mix = Gas_Liquid)	OUT	Anode Gas outflow
gas_out_Cat	Gas	(mix = Gas_Liquid)	OUT	Cathode Gas outflow
water_out	Water	(mix = Water)	OUT	Water outflow

A.3.27.4 Data

NAME	TYPE	DEFAULT	DESCRIPTION	UNITS
n_cell	INTEGER	15	Number of cells	-
A_cell	REAL	0.0175	Area of 1 cell	m^2
elp_a	REAL	0.2257	Coefficient to calculate the voltage	$V/(A/m^2)$
elp_b	REAL	0.07725	Coefficient to calculate the voltage	$V/(A^2/m^4)$
elp_c	REAL	0.01583	Coefficient to calculate the voltage	$V/(A^3/m^6)$
elp_d	REAL	0.00125	Coefficient to calculate the voltage	$V/(A^4/m^8)$
elp_T	REAL	0.0036	Coefficient to calculate the voltage	V/ºC
elp_TTref	REAL	355.2	Reference temperature in the voltage calculation	K
m_KOH	REAL	0.3	Mass of Electrolyte	kg
h_O2_Cat_dry	REAL	0.01	Molar fraction of oxygen in the dry gas cathode outlet	-
eff_f	REAL	1.0	Current or Faraday efficiency	-
T	REAL	350	Temperature in the electrolyser	K
Pr_Cat	REAL	10e5	Pressure in the Cathode gas outlet	Pa
Pr_An	REAL	10e5	Pressure in the Anode gas outlet	Pa
RH_Cat	REAL	0.9	Relative humidiy in the gas cathode	-
RH_An	REAL	0.9	Relative humidiy in the gas anode	-
I	REAL	37	Current or electrical electrisity	A

A.3.27.5 Variables

NAME	SYMBOL	TYPE	Description	Units
F	F= 96485	CONST REAL	Faraday's contant	Coulomb/mol
G_i	G[Process28]	REAL	Generation	mol/s
$H_{H2O,O2\_An}$	H_H2O_O2_An	REAL	Mols of H2O per mols of O2 in the anode gas outlet	
$H_{H2O,H2\_Cat}$	H_H2O_H2_Cat	REAL	Mols of H2O per mols of H2 in the cathode gas outlet	
I_D	I_D	REAL	Intensity density	$A/(m^2)$
P_{el}	P_el	REAL	Electrical power	W
R	R = 8.31434	CONST REAL	Ideal gas constant	$(Pa\ m^3)$ / (mol K)
TC	TC	REAL	Temperature in centigrade	ºC
U_{cell}	U_cell	REAL	Cell Voltage	V
U_{stack}	U_stack	REAL	Stack voltage	V
cm_{KOH}	cm_KOH	REAL	Mass concentration of KOH	-
Ze	z = 2	CONST REAL	Number of electrons reacting for one molecule of H_2	-
$Z_{H2O\ Lin}$	Z_in_H2O	REAL	Water molar inflow	mol/s
$Z_{H2O,Lout}$	Z_out_water[Process28]	REAL	Molar water outflow for each compound	mol/s
$Z_{i,Anout}$	Z_out_An[Process28]	REAL	Molar anode outflow for each compound	mol/s
$Z_{i,Catout}$	Z_out_Cat[Process28]	REAL	Molar cathode outflow for each compound	mol/s

A.3.27.6 Asserts

```
ASSERT ((TC> - 273.15 AND TC < 374.15)) WARNING \
            "Temperature out of range in H2O_psat Function"
```

A.3.27.7 Formulation

Details on mathematical model see chapter 4.6.1

A.3.28 Water Management Unit of ARES

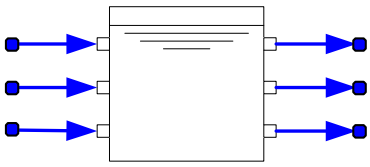
A.3.28.1 Description

This component type, named `Water_Management_ARES`, represents the processes of water collection and distribution in ARES. Thus, the recovered water from the CCA and CRA is part of the feed of the electrolyser and part of the steam necessary in the adsorber. Depending on the oxygen production and the quantity of carbon dioxide separated, additional water will be required.

The mathematic model allows obtaining the additional water necessary to fulfil the requirements specified

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.28.2 Symbol



Water_Management_ARES

A.3.28.3 Ports

NAME	TYPE	PARAMATERS	DIRECTION	DESCRIPTION
water_in_CCA	Liquid	(mix = Water)	IN	Water inflow from CCA
water_in_CRA	Liquid	(mix = Water)	IN	Water inflow from CRA
Water_in	Liquid	(mix = Water)	IN	Additional water inflow
water_out_CCA	Liquid	(mix = Water)	OUT	Water outflow towards CCA
Water_out	Liquid	(mix = Water)	OUT	Water non used
water_out_OGA	Liquid	(mix = Water)	OUT	Water outflow towards OGA

A.3.28.4 Data

NAME	TYPE	DEFAULT	DESCRIPTION	UNITS
Q_H2O_CCA	REAL	$5e^{-6}$	Volumetric flow of water necessary for the CCA	m^3/s
Q_H2O_OGA	REAL	$5e^{-2}$	Volumetric flow of water necessary for the OGA	m^3/s

A.3.28.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$Q_{H2O,ad}$	Q_H2O_ad	REAL	Water volumetric flow additional to achieve the requirements	m^3/s
$Q_{H2O,rec}$	Q_H2O_rec	REAL	Water volumetric inflow recovered	m^3/s
$Q_{H2O,req}$	Q_H2O_req	REAL	Water volumetric flow required for OGA and CCA	m^3/s
$W_{H2O,ad}$	W_H2O_ad	REAL	Water mass flow additional to achieve the requirements	kg/s

A.3.28.6 Formulation

Details on mathematical model see chapter 4.6.3

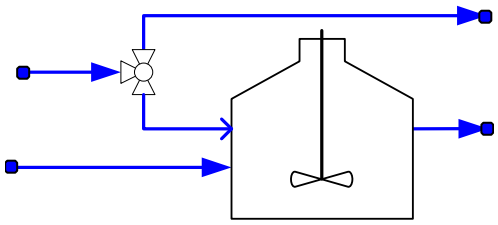
A.3.29 Dissolver of UTU

A.3.29.1 Description

This component type, named `Dissolver_UTU`, has to dilute the crew's urine. The nitrification process presents some restrictions in relation to the salts load. It is therefore important to dilute the urine (main source of salts) with water at the UTU's input. This dilution is also important for the nitrification process as it decreases the electro conductivity at the entry of the UTU system avoiding a decrease in the nitrification efficiency.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.29.2 Symbol



Dissolver_UTU

A.3.29.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`liq_in`	Liquid	`(mix=Urine_compounds)`	IN	Urine Inflow
`liq_out`	Liquid	`mix=Urine_compounds)`	OUT	Dissolved Urine Outflow
`water_in`	Liquid	`(mix=Water)`	IN	Water inflow
`water_out`	Liquid	`(mix=Water)`	OUT	Water outflow

A.3.29.4 Data

NAME	TYPE	DEFAULT	DESCRIPTION	UNITS
`R water urine`	REAL	1.4	Cubic meter of water per cubic meter of urine required to dilute urine at the desired conditions	-

A.3.29.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$Q_{H2O,ad}$	`Q_H2O_ad`	REAL	Volumetric flow of additional water	m^3/s
Z_{i,Lin_urine}	`Z_in_urine[Urine_compounds]`	REAL	Molar inflow of each urine compound at the urine inlet	mol/s
$Z_{H2O,ad}$	`Z_H2O_ad`	REAL	Molar inflow of additional water	mol/s

A.3.29.6 Formulation

Details on mathematical model see chapter 5.2.1

A.3.30 Urine Treatment Unit Bioreactor

A.3.30.1 Description

This component type, named `CIII_Bioreactor`, represents a nitrifying bioreactor and its function is to transform urea into nitrate.

The nitrification that takes place in this bioreactor is carried out by the same bacteria than colonize the nitrifying bioreactor of Compartment III of MELiSSA: the *Nitrobacter* and the *Nitrosomonas*. The process is similar and the same bioreactor can be used to treat the urine and the liquid coming from Compartment II of MELiSSA.

Thus, the formulation used for the UTU bioreactor is the same explained in Compartment III bioreactor, chapter 3.6.4 and 7.2A.3.3

A.3.31 Grey Water Treatment Unit

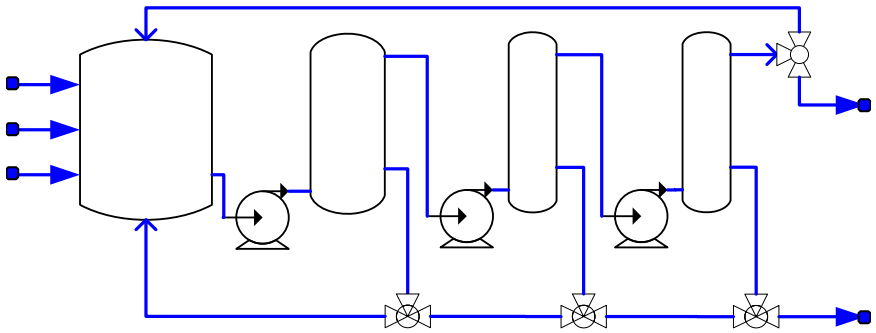
A.3.31.1 Description

This component type, named `Grey_Water_Treatment_Unit`, represents three successive membrane units: one nanofiltration unit based on a mineral membranes, and two reverse osmosis units. The role of the set of membranes is to recover hygienic water from the water coming from the crew chamber, from the condensate and from others subsystems, like UTU.

The mathematic model applied to this unit consists of calculating the recovered hygiene water.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.31.2 Symbol



Grey_Water_Treatment_Unit

A.3.31.3 Ports

NAME	TYPE	PARAMETERS	DIRECTION	DESCRIPTION
`water_crew_in`	Liquid	(mix=Water)	IN	Water inflow from the crew
`water_cond_in`	Liquid	(mix=Water)	IN	Condensate water inflow
`liq_in`	Liquid	(mix=Compounds)	IN	Liquid inflow from other subsystems
`water_hyg_out`	Liquid	(mix=Water)	OUT	Hygienic water outflow
`waste_out`	Liquid	(mix=Water)	OUT	Waste water outflow

A.3.31.4 Data

NAME	SYMBOL	TYPE	DEFAULT	DESCRIPTION	UNITS
R_{water}	`Rec_water`	REAL	0.9	Percentage of recovery from the total input	-

A.3.31.5 Variables

NAME	SYMBOL	TYPE	Description	Units
$Q_{Lin\ total}$	`Q_total_in`	REAL	Total volumetric inflow	m^3/s

A.3.31.6 Formulation

Details on mathematical model see chapter 6.2.1

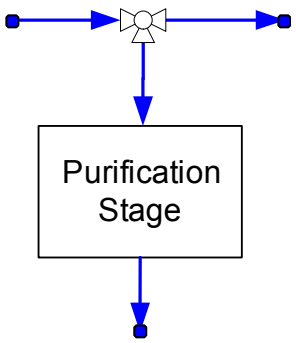
A.3.32 Water Potabiliser

A.3.32.1 Description

This component type, named `Water_Potabilizer`, represents the obtaining of potable water, as the hygiene water obtained through the GWTU is not potable and therefore needs further treatment to reach the level of potable water.

The mathematic description and assumptions are found in NTE-MEL2-TN-009.doc

A.3.32.2 Symbol



Water_Potabilizer

A.3.32.3 Ports

NAME	TYPE	DIRECTION	DESCRIPTION
`hyg_in`	Liquid (mix=Water)	IN	Hygiene water inflow
`hyg_out`	Liquid (mix=Water)	OUT	Hygiene water Outflow
`pot_out`	Liquid (mix=Water)	OUT	Potable water Outflow

A.3.32.4 Data

NAME	TYPE	DEFAULT	DESCRIPTION	UNITS
`Rec_pot`	REAL	0.9	percentage of potable water recovered from the total input	-

A.3.32.5 Formulation

Details on mathematical model see chapter 6.2.2