# **REACTION MECHANISM**

1. **Aerobic digestion** (Sole-Mauri et al., 2007)

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| **Hydrolysis phase by mesophilic bacterias** |
| Carbohydrates hydrolysis |
|
| Protein hydrolysis |
|
| Lipid hydrolysis |
|
| **Hydrolysis phase by thermophilic bacterias** |
| Carbohydrates hydrolysis |
|
| Protein hydrolysis |
|
| Lipid hydrolysis |
|
| **Thermophilic hydrolysis phase of macro-molecules** |
| Hydrolysis of hemicellulose by thermophilic actinomycetes |
|
| Hydrolysis of cellulose by thermophilic fungi |
|
| Hydrolysis of lignin by thermophilic fungi |
|
| **Mesophilic hydrolysis phase of macro-molecules** |
| Hydrolysis of hemicellulose by mesophilic actinomycetes |
|
| Hydrolysis of cellulose by mesophilic fungi |
|
| Hydrolysis of lignin by mesophilic fungi |
|
| **Growth of mesophilic bacterias** |
| Growth on |
|
| Growth on |
| Growth on |
| **Growth of thermophilic bacterias** |
| Growth on |
| Growth on |
| Growth on |
| **Growth of mesophilic actinomycetes** |
| Growth on |
| Growth on |
| Growth on |
| Growth on |
| **Growth of thermophilic actinomycetes** |
| Growth on |
| Growth on |
| Growth on |
| Growth on |
| **Growth of mesophilic fungi** |
| Growth on |
| Growth on |
| Growth on |
| Growth on |
| Growth on LG |
| **Growth of thermophilic fungi** |
| Growth on |
| Growth on |
| Growth on |
| Growth on |
| Growth on LG |
|  |

1. **Nitrification-Denitrification**
2. **Production of methane (Ge et al., 2016)**
3. **Death and lysis of heterotroph microorganisms**

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| **Nitrification** (Wang et al., 2009) |
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| **Denitrification** (Didier, 2013) |
| (Hypothèse : source de C très petite, et pas de variation de biomasse) |
| **Death and lysis of autotroph microorganisms** |
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| **Death of micro-organisms** |
| Death of MB |
| Death of TB |
| Death of MA |
| Death of TA |
| Death of MF |
| Death of TF |
| **Lysis of micro-organisms** |
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| **Hydrolysis** |
| Insoluble substrate Si: G, P, L, HE, CE |
| **Anaerobic digestion** |
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| **Oxidation of methane** |
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**State variables**

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| --- | --- | --- | --- |
| **Symbols** | **Units** | **Description** | **Formula** |
| G | kg/kgTM | Carbohydrates | C6H1206 |
| P | kg/kgTM | Proteins | C16H24O5N4 |
| L | kg/kgTM | Lipides | C25H45O3 |
| HE | kg/kgTM | Hemicelluloses | C10H18O9 |
| CE | kg/kgTM | Celluloses | (C6H12O6)n |
| LG | kg/kgTM | Lignines | C20H30O6 |
| Xi | kg/kgTM | Inert materials | C1.48H1.5O0.85N |
| Sc | kg/kgTM | Hydrolysis product of C and CE | C6H1206 |
| Sp | kg/kgTM | Hydrolysis product of P | C16H24O5N4 |
| Sl | kg/kgTM | Hydrolysis product of L | C25H45O3 |
| Sh | kg/kgTM | Hydrolysis product of H | C10H18O9 |
| Slg | kg/kgTM | Hydrolysis product of LG | C20H30O6 |
| Xmb | kg/kgTM | Mesophilic bacterias | C5H7O2N |
| Xtb | kg/kgTM | Thermophilic bacterias | C5H7O2N |
| Xma | kg/kgTM | Mesophilic actynomycetes | C5H7O2N |
| Xta | kg/kgTM | Thermophilic actynomycetes | C5H7O2N |
| Xmf | kg/kgTM | Mesophilic fungi | C10H17O6N |
| Xtf | kg/kgTM | Thermophilic fungi | C10H17O6N |
| Xa | kg/kgTM | autotroph microorganisms | C5H7O2N |
| Xdb | kg/kgTM | Decayed biomass | C5H7O2N |
| CO2 | kg/kgTM | Emission of CO2 gas |  |
| CH4 | kg/kgTM | Emission of CH4 gas |  |
| Sn | Kg/kgTM | Total dissolved ammonium (NH4+ - NH3) |  |
| NH3emitted | kg/kgTM | Emission of NH3 gas |  |
| NO3- | kg/kgTM | NO3- stock |  |
| N2 | kg/kgTM | Emission of N2 gas |  |
| N2O | kg/kgTM | Emission of N2O gas |  |
| H2O | kg/kgTM |  |  |
| T | K | Temperature of compost |  |
| So2 | mol/l | Concentration of oxygen in liquid phase |  |

**Parameters**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Parameters** | **Values** | **Unités** | **Signification** | **Ref** |
| k,h1C | 0,04 | h-1 | Mesophilic hydrolysis constant of carbohydrates (Xmb) | Sole-Mauri |
| k,h2P | 0,02 | h-1 | Mesophilic hydrolysis constant of proteins (Xmb) | Sole-Mauri |
| k,h3L | 0,01 | h-1 | Mesophilic hydrolysis constant of lipids (Xmb) | Sole-Mauri |
| k,h4C | 0,02 | h-1 | Thermophilic hydrolysis constant of carbohydrates (Xtb) | Sole-Mauri |
| k,h5P | 0,04 | h-1 | Thermophilic hydrolysis constant of proteins (Xtb) | Sole-Mauri |
| k,h6L | 0,01 | h-1 | Thermophilic hydrolysis constant of lipids (Xtb) | Sole-Mauri |
| k,h7H | 0,009 | h-1 | Thermophilic hydrolysis constant of hemicelluloses (Xta) | Sole-Mauri |
| k,h8CE | 0,007 | h-1 | Thermophilic hydrolysis constant of celluloses (Xtf) | Sole-Mauri |
| k,h9LG | 0,007 | h-1 | Thermophilic hydrolysis constant of lignins (Xtf) | Sole-Mauri |
| k,h10H | 0,009 | h-1 | Mesophilic hydrolysis constant of hemicelluloses (Xma) | Sole-Mauri |
| k,h11CE | 0,007 | h-1 | Mesophilic hydrolysis constant of celluloses (Xmf) | Sole-Mauri |
| k,h12LG | 0,007 | h-1 | Mesophilic hydrolysis constant of lignins (Xmf) | Sole-Mauri |
| khS | 1.00E-04 | kg/kg | Saturation coefficient for Contois kinetics : masse de substrat par masse de microorganisme | Sole-Mauri |
| µmb | 0,2 | h-1 | Specific growth rate for mesophilic bacteria on Sc, Sp, Sl | Sole-Mauri |
| µtb | 0,18 | h-1 | Specific growth rate for thermophilic bacteria on Sc, Sp, Sl | Sole-Mauri |
| µma | 0,1 | h-1 | Specific growth rate of mesophilic actinomycetes on Sc, Sp, Sl, Sh | Sole-Mauri |
| µta | 0,12 | h-1 | Specific growth rate of thermophilic actinomycetes on Sc, Sp, Sl, Sh | Sole-Mauri |
| µmf | 0,1 | h-1 | Specific growth rate of mesophilic fungi on Sc, Sp, Sl, Sh, Slg | Sole-Mauri |
| µtf | 0,1 | h-1 | Specific growth rate of thermophilic fungi on Sc, Sp, Sl, Sh, Slg | Sole-Mauri |
| µa | 0,03 | h-1 | Specific growth rate of autotroph microorganisms | Oudart |
| ks | 6.20E-05 | kg.dm-3 | Substrate saturation constant for Monod kinetics | Sole-Mauri |
| kNH4 | 5.00E-08 | kg.dm-3 | Ammonium saturation constant for heterotrophic activities | Sole-Mauri |
|  | 0.2.10-6 | mol/l | Oxygen saturation constant for heterotrophic activities | Sole-Mauri |
|  | 0.019.10-3 | mol/l | Oxygen saturation constant for nitrification | (Wang et al., 2009) |
|  | 8.4.10-2 | kg.dm-3 | Nitrate saturation constant for denitrification |  |
| bmb | 0,03 | h-1 | Death constant for mesophilic bacterias | Sole-Mauri |
| btb | 0,02 | h-1 | Death constant for thermophilic bacterias | Sole-Mauri |
| bma | 0,01 | h-1 | Death constant for mesophilic actinomycetes | Sole-Mauri |
| bta | 0,015 | h-1 | Death constant for thermophilic actinomycetes | Sole-Mauri |
| bmf | 0,01 | h-1 | Death constant for mesophilic fungis | Sole-Mauri |
| btf | 0,01 | h-1 | Death constant for thermophilic fungis | Sole-Mauri |
| ba | 0,0083 | h-1 | Death constant for autotroph microorganisms | Sole-Mauri |
| kdec | 0,0025 | h-1 | Microorganisms decomposition constant | Sole-Mauri |
| fi | 0,2 |  | Proportion of dead biomass recycled to inert materials | Oudart |
| pmaxdenit | 0.042 | kg-(N2O+N2)kg-1 NNO3 h-1 | Maximal emission of (N2O+N2) from NO3 denitrification | Oudart |
| pN2Odenit | 0.2 | kgN2ON/kg(N2O+N2)N | Proportion of N2O emission from denitrification | Oudart |
| YCH4,Sc | 0,267 | kgCH4/kgSc | Methane yield coefficient for carbohydrates | Theoric BMP |
| YCH4,Sp | 0.375 | kgCH4/kgSp | Methane yield coefficient for proteins | Theoric BMP |
| YCH4,Sl | 0.707 | kgCH4/kgSl | Methane yield coefficient for lipids | Theoric BMP |
| YCH4,Sh | 0.284 | kgCH4/kgSh | Methane yield coefficient for hemicelluloses | Theoric BMP |
| YCH4,Slg | 0.535 | kgCH4/kgSlg | Methane yield coefficient for lignin | Theoric BMP |
|  | 400.103 | l.mol-1 | Sensibilité de la méthanogénèse à l’inhibition par l’oxygène |  |
| Km | 0.045 | molCH4.m-3 IW | Half saturation constant for methane in methane oxidation | Watson et al., 1997) |
| 0.72 | kgCH4/l |  |
| Ko2 | 0.033 | molO2.m-3 IW | Half saturation constant for oxygen in methane oxidation | (Watson et al., 1997) |
| 0.033. 10-3 | Mol/l |  |
| Vmax | Between 2.6 and 4.1 | µmolCH4.g-1 of dw.h-1 | Maximum methane oxidation potential | (JÃ¤ckel et al., 2005) |
| 1.152.10-4 | kgCH4.kgTM-1.h-1 | \*the compost is very mature (5 years) | (Yuan et al., 2009) |
| 5.352.10-4 | kgCH4.kgTM-1.h-1 | \*compost of MSW 184 days | (Wilshusen et al., 2004) |
| 0.0205 | molCH4.kg-1VSaero.h-1 | Maximum methane oxidation (VS aero 🡪? : difficile à utiliser) | (Ge et al., 2016) |
|  |  | - | Concentration of oxygen in gas phase | (Jiang et al., 2015) |
|  | 0.00126 | mol.l-1.atm-1 | Reference Henry constant |  |
| Yo2 |  | Mol.mol-1 | Biomass yield on oxygen |  |

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