**Supplementary Data (SD) for**

**A plant-wide energy model for WWTPs: application to AnMBR technology**

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**Table S1.** Standard molar enthalpy of formation (ΔHºF) at 298K in Kcal·mol-1 and coefficients (A, B, C, D y E) of the molar heat capacity at constant pressure [36] for solids, liquids and gaseous substances in BNRM2.

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**Figure S1**. Example of a window extracted from the energy tool included in DESASS: **(a)** design properties of the gas blower; and **(b)** design properties of the anaerobic MBR.

**Table S1**.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Solids and liquids substances** | **ΔHºF, Kcal·mol-1** | **A** | **B** | **C** | **D** | **E** |
| **CH4(l)** | -17.79 | 6.5708x101 | 3.8883x104 | -2.5795x102 | 6.1407x102 | --- |
| **C2H4O2(l)** | -103.37 | 1.3964x105 | -3.2080x102 | 8.9850x10-1 | --- | --- |
| **C3H6O2(l)** | -108.31 | 2.1366x105 | -7.0270x102 | 1.6605 | --- | --- |
| **C4H6O2(s)** | -54.21 | 1.1600x105 | --- | --- | --- | --- |
| **C6H10O5(s)** | -244.09 | 2.08x105 | --- | --- | --- | --- |
| **C12H22O11(l)** | -530.62 | 2.6565x105 | 6.9779x102 | --- | --- | --- |
| **CO2(l)** | -94.05 | -8.3043x106 | 1.0437x105 | -4.3333x102 | 6.0052x10-1 |  |
| **HNO3(l)** | -32.07 | 1.3125x105 | -1.2190x102 | 1.7040x10-1 | --- | --- |
| **H2CO3(l)** | -146.64 | 5.5x102 | 4.27x102 | --- | --- | --- |
| **H2(l)** | --- | 2.256x104 | -1.9859x103 | 1.1547x102 | -1.2598 |  |
| **H2O(l)** | -57.8 | 2.7637x105 | -2.0901x103 | 8.1250 | -1.4116x10-2 | 9.3701x10-6 |
| **H2SO4(l)** | -175.57 | 5.983x104 | 3.9520x102 | -5.2067x10-1 | 3.1220x10-4 | -7.0570x10-8 |
| **H2S(l)** | -4.92 | -3.749x106 | -5.5411x104 | 2.7765x102 | -4.631x10-1 | --- |
| **H3PO4(l)** | -299.54 | 5.5228x104 | 3.0125x102 | --- | --- | --- |
| **HPO3(s)** | 8.3532 | 41.727 | 0.3925 | -0.0003 | --- | --- |
| **NH4(l)** | -10.96 | 3.0094x106 | -4.3692x104 | 2.4114x102 | -5.8560x10-1 | 5.2953x10-4 |
| **NO2(l)** | 4.924 | 9.1934x104 | 1.7086x102 | -4.3000x10-3 | --- | --- |
| **N2(l)** | --- | -3.34x104 | 3.507x103 | -4.67x101 | 2.127x10-1 | --- |
| **O2(l)** | --- | 6.8337x104 | -6.1354x102 | 7.928 | -3.168x10-2 | --- |
| **Gaseous substances** |  |  |  |  |  |  |
| **H2S(g)** | -4.92 | 3.3288x104 | 2.6086x104 | 9.1340x102 | -1.7979x104 | 9.4940x102 |
| **N2(g)** | --- | 2.9105x104 | 8.6149x103 | 1.7016x103 | 1.0347x102 | 9.0979x102 |
| **CO2(g)** | -94.05 | 2.937x104 | 3.454x104 | -1.428x103 | 2.6400x104 | 5.88x102 |
| **CH4(g)** | -17.79 | 3.3298x104 | 7.9933x104 | 2.0869x103 | 4.1602x104 | 9.9196x102 |
| **H2(g)** | --- | 2.7617x104 | 9.5600x103 | 2.466x103 | 3.7600x103 | 5.6760x102 |
| **NH3(g)** | -10.96 | 3.3480x104 | 4.8200x104 | 9.5189x102 | -3.0100x104 | 1.0560x103 |
| **O2(g)** | --- | 2.9103x104 | 1.0040x104 | 2.5265x103 | 9.356x103 | 1.1538x103 |



**(a)**



**(b)**

**Figure S1.**