Supplementary file

Investigation on the effects of solvent selection towards dissolution of waste plastics

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**Table S1**. Hansen & Hildebrand solubility parameters of polymers & solvents

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Polymers** | | | | | |
| **Material** | **δD** | **δP** | **δH** | **δ1** | **Interaction radius** |
| **Mpa0.5** | **Mpa0.5** | **Mpa0.5** | **Mpa0.5** | **R0** |
| Polystyrene (PS) | 18.5 | 4.5 | 2.9 | 19.3 | 5.3 |
| Polypropylene (PP) | 18 | 0 | 1 | 18.0 | 6 |
| Polyethylene - High Density (HDPE) | 16 | 0.8 | 2.8 | 16.3 | 3.2 |
| Acrylonitrile - Butadiene - Styrene (ABS) | 16.3 | 2.7 | 7.1 | 17.98 | 7.8 |
| **Solvents** | | | | | |
| Acetone | 15.5 | 10.4 | 7 | 19.9 | 74 |
| Acetonitrile | 15.3 | 18 | 6.1 | 24.4 | 52.6 |
| Benzene | 18.4 | 0 | 2 | 18.5 | 89.4 |
| Chloroform | 17.8 | 3.1 | 5.7 | 18.9 | 80.7 |
| m-Cresol | 18 | 5.1 | 12.9 | 22.7 | 104.7 |
| Cyclohexanol | 17.4 | 4.1 | 13.5 | 22.4 | 106 |
| Cyclohexanone | 17.8 | 6.3 | 5.1 | 19.6 | 104 |
| 1,2 Dichlorobenze | 19.2 | 6.3 | 3.3 | 20.5 | 112.8 |
| Dichloromethane | 18.2 | 6.3 | 6.1 | 20.2 | N/A |
| Dimethylformamide | 17.4 | 13.7 | 11.3 | 24.9 | 77 |
| Ethanol | 15.8 | 8.8 | 19.4 | 26.5 | 58.5 |
| Ethyl acetate | 15.8 | 5.3 | 7.2 | 18.2 | 98.5 |
| Heptane | 15.3 | 0 | 0 | 15.3 | 147.4 |
| Hexadecane | 16.3 | 0 | 0 | 16.3 | 294.1 |
| Hexafluoro-2-propanol | 17.2 | 4.5 | 14.7 | 23.1 | 105.3 |
| Hexane | 14.9 | 0 | 0 | 14.9 | 131.6 |
| Methanol | 15.1 | 12.3 | 22.3 | 29.6 | 40.7 |
| Methyl Ethyl Ketone | 16 | 9 | 5.1 | 19.1 | 90.1 |
| Tetrahydrofuran | 16.8 | 5.7 | 8 | 19.5 | 81.7 |
| Toluene | 18 | 1.4 | 2 | 18.2 | 106.8 |
| Xylene | 17.6 | 1 | 3.1 | 17.9 | 123.3 |

**Table S2.** Solvents' distance from the centre for the RED method

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Distance from the Centre** | | | | |
| **Ra** | **PS** | **PP** | **HDPE** | **ABS** |
| Acetone | 9.4 | 13.0 | 10.5 | 7.9 |
| Acetonitrile | 15.3 | 19.5 | 17.6 | 15.5 |
| Benzene | 4.6 | 1.3 | 4.9 | 7.1 |
| Chloroform | 3.4 | 5.6 | 5.2 | 3.3 |
| m-Cresol | 10.1 | 12.9 | 11.7 | 7.1 |
| Cyclohexanol | 10.8 | 13.2 | 11.5 | 6.9 |
| Cyclohexanone | 3.2 | 7.5 | 7.0 | 5.1 |
| 1,2 Dichlorobenze | 2.3 | 7.1 | 8.5 | 7.8 |
| Dichloromethane | 3.7 | 8.1 | 7.8 | 5.3 |
| Dimethylformamide | 12.7 | 17.2 | 15.7 | 12.0 |
| Ethanol | 17.9 | 20.9 | 18.4 | 13.8 |
| Ethyl acetate | 6.9 | 9.3 | 6.3 | 2.8 |
| Heptane | 8.3 | 5.5 | 3.2 | 7.9 |
| Hexadecane | 6.9 | 3.5 | 3.0 | 7.6 |
| Hexafluoro-2-propanol | 12.1 | 14.5 | 12.7 | 8.0 |
| Hexane | 9.0 | 6.3 | 3.6 | 8.1 |
| Methanol | 22.0 | 25.3 | 22.7 | 18.1 |
| Methyl Ethyl Ketone | 7.1 | 10.7 | 8.5 | 6.6 |
| Tetrahydrofuran | 6.2 | 9.3 | 7.3 | 3.3 |
| Toluene | 3.4 | 1.7 | 4.1 | 6.3 |
| Xylene | 3.9 | 2.5 | 3.2 | 5.1 |
| 15% Acetonitrile 85% Toluene | 1.9 | 4.3 | 4.4 | 5.3 |
| 40% Cyclohexanone 60% Toluene | 4.5 | 1.3 | 3.4 | 6.6 |
| 50% Cyclohexanone 50% Xylene | 2 | 5.7 | 5.3 | 4.6 |
| 80% Cyclohexane 20% Cyclohexanol | 4.9 | 3 | 1.8 | 4.8 |
| 87% Cyclohexanol 13% Ethanol | 11.7 | 14.2 | 12.3 | 7.7 |
| 25% Heptane 75% Xylene | 4.8 | 2.5 | 2.1 | 5.4 |
| 25% Cyclohexane 75% Toluene | 4 | 1.3 | 3.6 | 6.4 |
| 40% Cyclohexane 60% Xylene | 4.7 | 1.8 | 2.7 | 5.9 |

**Table S3.** Flory-Huggins parameters of selected solvents

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Solvent** | **V(cm3/mol)** | **A1,2** | | | |
| **PS** | **PP** | **HDPE** | **ABS** |
| Acetone | 74 | 21.9 | 42.3 | 27.7 | 15.5 |
| Acetonitrile | 100 | 58.4 | 94.8 | 77.2 | 59.8 |
| Benzene | 89.4 | 5.3 | 0.4 | 6.1 | 12.7 |
| Chloroform | 80.7 | 2.9 | 8.0 | 6.7 | 2.8 |
| m-Cresol | 100 | 25.3 | 41.9 | 34.1 | 12.7 |
| Cyclohexanol | 100 | 29.3 | 43.6 | 33.3 | 11.9 |
| Cyclohexanone | 104 | 2.5 | 14.2 | 12.1 | 6.5 |
| 1,2 Dichlorobenze | 100 | 1.3 | 12.7 | 17.9 | 15.3 |
| Dichloromethane | 100 | 3.5 | 16.5 | 15.1 | 7.1 |
| Dimethylformamide | 100 | 40.0 | 73.8 | 61.6 | 35.9 |
| Ethanol | 100 | 80.0 | 108.8 | 84.9 | 47.4 |
| Ethyl Acetate | 98.5 | 12.1 | 21.5 | 9.9 | 1.9 |
| Heptane | 100 | 17.4 | 7.5 | 2.6 | 15.4 |
| Hexadecane | 100 | 12.0 | 3.1 | 2.2 | 14.4 |
| Hexafluoro-2-propanol | 100 | 36.5 | 52.6 | 40.3 | 16.1 |
| Hexane | 131.6 | 20.1 | 9.9 | 3.3 | 16.4 |
| Methanol | 40.7 | 120.9 | 159.7 | 128.9 | 82.2 |
| Methyl Ethyl Ketone | 90.1 | 12.5 | 28.5 | 18.1 | 11.0 |
| Tetrahydrofuran | 100 | 9.8 | 21.8 | 13.4 | 2.7 |
| Toluene | 106.8 | 2.9 | 0.7 | 4.3 | 9.8 |
| Xylene | 123.3 | 3.9 | 1.5 | 2.6 | 6.4 |

**Table S4.** Fractional parameters of plastics & polymers for the creation of the Teas graph

|  |  |  |  |
| --- | --- | --- | --- |
| **Polymers / Solvents** | **FD** | **FP** | **FH** |
| Polystyrene (P1) | 71.4 | 17.4 | 11.2 |
| Polypropylene (P2) | 94.7 | 0.0 | 5.3 |
| Polyethylene - High Density (P3) | 81.6 | 4.1 | 14.3 |
| Acrylonitrile - Butadiene - Styrene (P4) | 62.5 | 10.3 | 27.2 |
| Acetone (S1) | 47.1 | 31.6 | 21.3 |
| Acetonitrile (S2) | 38.8 | 45.7 | 15.5 |
| Benzene (S3) | 90.2 | 0.0 | 9.8 |
| Chloroform (S4) | 66.9 | 11.7 | 21.4 |
| m-Cresol (S5) | 50.0 | 14.2 | 35.8 |
| Cyclohexanol (S6) | 49.7 | 11.7 | 38.6 |
| Cyclohexanone (S7) | 61.0 | 21.6 | 17.5 |
| 1,2 Dichlorobenzene (S8) | 66.7 | 21.9 | 11.5 |
| Dichloromethane (S9) | 59.5 | 20.6 | 19.9 |
| Dimethylformamide (S10) | 41.0 | 32.3 | 26.7 |
| Ethanol (S11) | 35.9 | 20.0 | 44.1 |
| Ethyl acetate (S12 | 55.8 | 18.7 | 25.4 |
| Heptane (S13) | 100.0 | 0.0 | 0.0 |
| Hexadecane (S14) | 100.0 | 0.0 | 0.0 |
| Hexafluoro-2-propanol (S15) | 47.3 | 12.4 | 40.4 |
| Hexane (S16) | 100.0 | 0.0 | 0.0 |
| Methanol (S17) | 30.4 | 24.7 | 44.9 |
| Methyl Ethyl Ketone (S18) | 53.2 | 29.9 | 16.9 |
| Tetrahydrofuran (S19) | 55.1 | 18.7 | 26.2 |
| Toluene (S20) | 84.1 | 6.5 | 9.3 |
| Xylene (S21) | 81.1 | 4.6 | 14.3 |