

Life cycle assessment of multistep benzoxazoles synthesis: from batch to waste-minimized continuous flow systems

Jose Osorio-Tejada,^a Francesco Ferlin,^b Luigi Vaccaro,^b Volker Hessel,^{a,c}

^a Department of Chemical Engineering, School of Engineering, University of Warwick, Coventry, UK

^b Laboratory of Green S.O.C. – Dipartimento di Chimica, biologia e Biotecnologie, Università degli Studi di Perugia, Via Elce di Sotto 8, 06123 – Perugia, Italy. E-mail: luigi.vaccaro@unipg.it; <http://greensoc.chm.unipg.it/>.

^c School of Chemical Engineering and Advanced Materials, University of Adelaide, Adelaide, Australia

Electronic Supplementary Information (ESI)

LCA INVENTORIES DATASET

Inventories for the nine benchmarked synthesis processes

Table 1. CF approach OMS multigram scale

| Inputs | Quantity for 53.5 g of product ¹ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------------------|---|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Benzyl alcohol | 33.3 g | 6.22E-01 g | 1.24E-03 | 7.66E-02 | 6.52E-03 | 6.97E-03 |
| CPME (cyclopentyl methyl ether) | 610 g | 2.28E-01 g | 2.28E-02 | 3.43E-01 | 1.99E-02 | 5.36E-02 |
| o-aminophenol | 30.5 g | 5.70E-01 g | 0 | 1.73E-02 | 1.09E-03 | 2.94E-03 |
| K-OMS | 68 mg | 2.54E-08 g | 0 | 0 | 1.27E-08 | 1.27E-08 |
| H-OMS | 78 mg | 2.92E-08 g | 0 | 0 | 1.46E-08 | 1.46E-08 |
| O ₂ (3.88 L of gas) | 5.5 g | 1.04E-01 g | 0 | 0 | 0 | 0.00E+00 |
| N ₂ (3.02 L of gas) | 3.8 g | 7.06E-02 g | 0 | 0 | 0 | 0.00E+00 |
| Ethanol | 71 g | 3.85E-01 g | 2.65E-03 | 4.63E-01 | 3.71E-02 | 9.98E-02 |
| Heating at 106 °C for 24 h | | 2.43E-02 kWh | | | | |
| Energy to recover solvents | | 3.03E-03 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 2. CF approach OMS small scale

| Inputs | Quantity for 0.708 g of product ¹ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|--------------------------------|--|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Benzyl alcohol | 0.432 g | 6.10E-01 g | 1.22E-03 | 9.95E-02 | 5.34E-03 | 1.44E-02 |
| CPME | 24 g | 6.78E-01 g | 6.78E-02 | 1.02E+00 | 5.92E-02 | 1.59E-01 |
| o-aminophenol | 0.404 g | 5.71E-01 g | | 1.81E-02 | 1.14E-03 | 3.07E-03 |
| K-OMS | 68 mg | 1.92E-06 g | | 0 | 9.60E-07 | 9.60E-07 |
| H-OMS | 78 mg | 2.20E-06 g | | 0 | 1.10E-06 | 1.10E-06 |
| O ₂ (3.88 L of gas) | 0.08 g | 1.12E-01 g | | | | |
| N ₂ (3.02 L of gas) | 0.05 g | 7.62E-02 g | | | | |
| Ethanol | 3.90 g | 1.60E+00 g | 1.10E-02 | 1.92E+00 | 1.54E-01 | 4.14E-01 |
| Heating at 106 °C for 58 min | | 6.28E-03 kWh | | | | |
| Energy to recover solvents | | 9.77E-03 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 3. Batch approach OMS

| Inputs | Quantity for 0.037 g of product ¹ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|--------------------------------|--|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Benzyl alcohol | 0.043 g | 1.16E+00 g | 2.32E-03 | 1.10E+00 | 5.88E-02 | 1.58E-01 |
| CPME | 5.16 g | 2.79E+00 g | 2.79E-01 | 4.20E+00 | 2.43E-01 | 6.56E-01 |
| o-aminophenol | 0.022 g | 5.95E-01 g | | 5.49E-02 | 3.47E-03 | 9.34E-03 |
| K-OMS | 17.7 g | 9.57E-06 g | | | 4.78E-06 | 4.78E-06 |
| H-OMS | 35.4 g | 1.91E-05 g | | | 9.57E-06 | 9.57E-06 |
| O ₂ | | | | | | |
| N ₂ | | | | | | |
| Ethanol | 3.90 g | 1.24E+01 g | 8.54E-02 | 1.49E+01 | 1.19E+00 | 3.21E+00 |
| Heat (106 °C for 70 min) | | 6.05E-02 kWh | | | | |
| Energy to recover solvents | | 5.00E-02 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |
| Energy to regenerate catalysts | | 7.74E-02 kWh | | | | |

Table 4. Batch approach via dichlorodicyanobenzoquinone (DDQ) - Chang et al. 2002

| Inputs | Quantity for 0.181 g of product ² | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|-------------------------------------|--|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| o-aminophenol | 0.109 g | 6.02E-01 g | | 6.66E-02 | 4.21E-03 | 1.13E-02 |
| Methanol | 3.9 g | 6.25E+00 g | 4.31E-02 | 5.42E+00 | 6.02E-01 | 1.62E+00 |
| Benzaldehyde | 0.106 g | 5.86E-01 g | 1.17E-03 | 7.55E-02 | 3.97E-03 | 1.07E-02 |
| Dichloromethane | 26.6 g | 4.26E+01 g | 2.94E-01 | 13.9E+00 | 4.11E+00 | 1.11E+01 |
| DDQ | 0.25 g | 1.38E+00 g | | | 1.38E+00 | |
| Saturated Sodium carbonate | 22 g | 1.22E+02 g | | | 1.22E+02 | |
| Brine | 11.5 g | 6.35E+01 g | | | 6.35E+01 | |
| Ethyl acetate in chrom. column | 0.016 g | 9.02E-02 g | 1.80E-04 | 1.14E-01 | 8.73E-03 | 2.35E-02 |
| Hexane in chrom. column | 0.1067 g | 5.90E-01 g | 1.18E-03 | 1.14E+00 | 5.71E-02 | 1.54E-01 |
| Heat (45 °C 12 h) and stir (30 min) | | 3.24E-02 kWh | | | | |
| Energy to recover solvents | | 4.25E-02 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 5. Batch approach via phosphonium acidic ionic liquid - Nguyen et al. 2018

| Inputs | Quantity for 0.177 g of product ³ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|----------------------------------|--|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| o-aminophenol | 0.109 g | 6.16E-01 g | | 8.75E-02 | 5.53E-03 | 1.49E-02 |
| Benzaldehyde | 0.106 g | 5.99E-01 g | 1.20E-03 | 9.99E-02 | 5.26E-03 | 1.42E-02 |
| Phosphonium acidic ionic liquid | 0.0205 g | 2.90E-02 g | | 4.26E-02 | 2.81E-03 | 7.56E-03 |
| Diethyl ether (10 x 5 mL) | 35.6 g | 5.83E+01 g | 4.02E-01 | 8.73E+01 | 5.62E+00 | 1.51E+01 |
| Acetone in chrom. column | 0.007 g | 3.92E-02 g | 7.84E-05 | 5.64E-02 | 3.79E-03 | 1.02E-02 |
| Petroleum Ether in chrom. column | 0.108 g | 6.08E-01 g | 1.22E-03 | 1.18E+00 | 5.89E-02 | 1.59E-01 |
| Heat and stir (100 °C 30 min) | | 8.78E-04 kWh | | | | |
| Energy to recover Phosphonium | | 3.78E-02 kWh | | | | |
| Energy to recover solvents | | 3.78E-02 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 6. Batch approach via Ru-catalysed ADC reactions - Khalafi & Panahi 2014

| Inputs | Quantity for 0.152 g of product ⁴ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---|--|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| o-aminophenol | 0.109 g | 7.17E-01 g | | 2.43E-01 | 1.54E-02 | 4.13E-02 |
| Benzyl alcohol | 0.112 g | 7.37E-01 g | 1.47E-03 | 3.28E-01 | 1.76E-02 | 4.74E-02 |
| Toluene | 2.6 g | 4.96E+00 g | 3.42E-02 | 1.05E+01 | 4.78E-01 | 1.29E+00 |
| DABCO | 0.06 g | 3.95E-01 g | 7.89E-04 | 5.89E-01 | 3.82E-02 | 1.03E-01 |
| PFMN ligand | 0.05 g | | | | | |
| Ru ₂ Cl ₄ (CO) ₆ | 0.01 g | 1.10E-02 g | | | 1.10E-02 | |
| Diethyl ether | 21.4 g | 4.08E+01 g | 2.82E-01 | 6.11E+01 | 3.93E+00 | 1.06E+01 |
| Ethyl acetate in chrom. column | 0.069 g | 4.51E-01 g | 9.02E-04 | 5.71E-01 | 4.37E-02 | 1.18E-01 |
| Petroleum Ether in chrom. column | 0.0486 g | 3.20E-01 g | 6.40E-04 | 6.21E-01 | 3.10E-02 | 8.34E-02 |
| Heat (110 °C 24 h) | | 2.62E-01 kWh | | | | |
| Energy to recover solvents | | 4.26E-02 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 7. Batch approach via CuO nanoparticles - Saha et al. 2009

| Inputs | Quantity for 0.186 g of product ⁵ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---|--|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| N-(2-bromophenyl) benzamide | 0.27613 g | 1.48E+00 g | | 9.22E-02 | 6.80E-03 | 1.83E-02 |
| Copper Oxide (CuO) Nanoparticles | 0.004 g | 4.30E-04 g | | | 1.08E-04 | 1.28E-04 |
| Potassium carbonate (K ₂ CO ₃) | 0.207 g | 1.11E+00 g | | | 1.11E+00 | |
| DMSO (1mL) | 1.1 g | 1.72E+00 g | 1.18E-02 | 1.22E+00 | 1.65E-01 | 4.45E-01 |
| Ethyl acetate (20 mL) | 18.04 g | 2.81E+01 g | 1.94E-01 | 3.54E+01 | 2.71E+00 | 7.30E+00 |
| Brine (1x 5mL) | 6.01 g | 3.23E+01 g | 6.46E-02 | | 3.22E+01 | |
| Water (2 x 5 mL) | 10 g | 5.38E+01 g | 1.08E-01 | | 4.83E+01 | |
| Ethyl acetate in chrom. column | 0.084 g | 4.51E-01 g | 9.02E-04 | 5.71E-01 | 4.37E-02 | 1.18E-01 |
| Hexane in chrom. column | 0.0609 g | 3.28E-01 g | 6.55E-04 | 6.36E-01 | 3.17E-02 | 8.54E-02 |
| Heat and stir (110 °C 16 h) | | 1.24E-01 kWh | | | | |
| Energy to recover solvents | | 2.36E-02 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 8. Batch approach via Pyridine-chlorochromate (PCC) - Praveen et al. 2008

| Inputs | Quantity for 0.3551 g of product ⁶ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|----------------------------------|---|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Schiff's base | 0.42628 g | 1.20E+00 g | | 1.84E-01 | 1.05E-02 | 2.83E-02 |
| Silica supported PCC | 0.47423 g | 1.34E+00 g | | | 6.68E-01 | 2.65E-01 |
| Dichloromethane (10 ml) | 13.25 g | 1.08E+01 g | 7.46E-02 | 3.54E+00 | 1.04E+00 | 2.81E+00 |
| Ethyl acetate (3x20 mL). | 54.12 g | 4.42E+01 g | 3.05E-01 | 5.57E+01 | 4.26E+00 | 1.15E+01 |
| Ethyl acetate in chrom. column | 0.160 g | 4.51E-01 g | 9.02E-04 | 5.71E-01 | 4.37E-02 | 1.18E-01 |
| Petroleum Ether in chrom. column | 0.1136 g | 3.20E-01 g | 6.40E-04 | 6.21E-01 | 3.10E-02 | 8.34E-02 |
| Stir (30 min) | | 1.95E-02 kWh | | | | |
| Energy to recover solvents | | 3.85E-02 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Table 9. Batch approach via acyl chloride - Wang et al. 2013

| Inputs | Quantity for 0.0319 g of product ⁷ | Quantity for 1 g of product | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|----------------------------------|---|-----------------------------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| benzo[d]oxazole (0.2 mmol) | 0.02382 g | 7.47E-01 g | | 2.25E-01 | 1.33E-02 | 3.57E-02 |
| Acyl chloride (0.4mmol) | 0.03140 g | 2.85E-01 g | 1.97E-03 | 2.02E-01 | 2.75E-02 | 7.40E-02 |
| Potassium carbonate ((0.2 mmol) | 0.02764 g | 8.66E-01 g | | | 8.66E-01 | |
| PhCl (0.3 mL) | 0.3318 g | 3.02E+00 g | 2.08E-02 | 4.46E+00 | 2.91E-01 | 7.83E-01 |
| H2O (0.1mL) | 0.1 g | 3.13E+00 g | 6.27E-03 | | 2.82E+00 | |
| Ethyl acetate in chrom. column | 0.014 g | 4.51E-01 g | 9.02E-04 | 5.71E-01 | 4.37E-02 | 1.18E-01 |
| Petroleum Ether in chrom. column | 0.0102 g | 3.20E-01 g | 6.40E-04 | 6.21E-01 | 3.10E-02 | 8.34E-02 |
| Heat and stir (140 °C 12h) | | 2.87E-01 kWh | | | | |
| Energy to recover solvents | | 6.49E-03 kWh | | | | |
| Chemical factory | | 4.00E-13 unit | | | | |

Inventories for the needed compounds in the synthesis approaches that were not available in life cycle databases

The development of these inventories was based on data from experimental sections in literature. When the yield of the synthesis was not stated, we assumed 95% yields.

Table 10. CPME

| Inputs | Quantity for 1 g of product | | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------|-----------------------------|------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Cyclopentene | 7.16E-01 | g | 1.43E-03 | 7.05E-02 | 3.33E-03 | 8.97E-03 |
| Methanol | 3.37E-01 | g | 6.73E-04 | 1.41E-02 | 1.57E-03 | 4.22E-03 |
| Sulfuric acid | 7.00E-01 | g | | | *5.07E-01 | |
| Heating steam | 2.00E-03 | MJ | | | | |
| Electricity | 3.33E-04 | kWh | | | | |
| Chemical factory | 4.00E-13 | unit | | | | |
| Transport lorry>16t | 1.00E-04 | tkm | | | | |
| Transport train | 6.00E-04 | tkm | | | | |

*Neutralized. It goes to water in form of NaSO₄

Table 11. H-OMS

| Inputs | Quantity for 1 g of product | | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------|-----------------------------|------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| K-OMS | 1.11E+00 | g | | | 5.56E-02 | 5.56E-02 |
| Nitric acid | 1.57E+01 | g | | | *2.12E+01 | |
| Deionized water | 1.11E+02 | g | 2.22E-01 | | 9.96E+01 | |
| Heating steam | 2.00E-03 | MJ | | | | |
| Electricity | 3.33E-04 | kWh | | | | |
| Chemical factory | 4.00E-13 | unit | | | | |
| Transport lorry>16t | 1.00E-04 | tkm | | | | |
| Transport train | 6.00E-04 | tkm | | | | |

*Neutralized. It goes to water in form of NaNO₃

Table 12. K-OMS

| Inputs | Quantity for 1 g of product | | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|----------------------------|-----------------------------|------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Manganese sulphate hydrate | 1.05E+00 | g | | | 5.24E-02 | 5.24E-02 |
| Nitric acid | 5.05E-01 | g | | | *6.81E-01 | |
| Deionized water | 6.06E+01 | g | 1.21E-01 | | 5.45E+01 | |
| Potassium permanganate | 6.90E-01 | g | | | 6.90E-02 | |
| Heating steam | 2.00E-03 | MJ | | | | |
| Electricity | 3.33E-04 | kWh | | | | |
| Chemical factory | 4.00E-13 | unit | | | | |
| Transport lorry>16t | 1.00E-04 | tkm | | | | |
| Transport train | 6.00E-04 | tkm | | | | |

*Neutralized. It goes to water in form of NaNO₃

Table 13. DDQ

| Inputs | Quantity for 1 g of product ⁸ | | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|--------------------------------------|--|------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| 2,3-dicyanohydroquinone (DCH) | 7.80E-01 | g | | 1.04E-01 | 7.25E-03 | 1.95E-02 |
| Water | 5.46E+00 | g | 8E-13 | 4.91E-01 | 4.91E+00 | |
| Concentrated nitric acid (70%) | 1.47E+00 | g | | | *2.83E+00 | |
| Concentrated hydrochloric acid (30%) | 6.49E+00 | g | | | **1.04E+01 | |
| Carbon tetrachloride | 8.00E-01 | g | | | 8.00E-01 | |
| Heating steam | 2.00E-03 | MJ | | | | |
| Electricity | 3.33E-04 | kWh | | | | |
| Chemical factory | 4.00E-13 | unit | | | | |
| Transport lorry>16t | 1.00E-04 | tkm | | | | |
| Transport train | 6.00E-04 | tkm | | | | |

*Neutralized. It goes to water in form of NaNO₃. **Neutralized. It goes to water in form of NaCl

Table 14. Phosphonium acidic ionic

| Inputs | Quantity for 1 g of product ³ | | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|------------------------|--|------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Triphenylphosphine | 4.74E-01 | g | | 2.73E-02 | 1.38E-03 | 3.72E-03 |
| 1,4-butane sultone | 2.46E-01 | g | | 6.08E-03 | 7.18E-04 | 1.93E-03 |
| Toluene solvent | 2.51E+00 | g | 5.03E-03 | 5.33E+00 | 2.43E-01 | 6.55E-01 |
| p-toluenesulfonic acid | 3.11E-01 | g | | 1.06E-02 | 9.02E-04 | 2.43E-03 |
| Diethyl ether | 2.07E+01 | g | 4.14E-02 | 3.11E+01 | 2.00E+00 | 5.39E+00 |
| Heating steam | 2.00E-03 | MJ | | | | |
| Electricity | 3.33E-04 | kWh | | | | |
| Chemical factory | 4.00E-13 | unit | | | | |
| Transport lorry>16t | 1.00E-04 | tkm | | | | |
| Transport train | 6.00E-04 | tkm | | | | |

Table 15. DABCO (triethylenediamine)

| Inputs | Quantity for 1 g of product ⁹ | | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|----------------------------------|--|------|---------------------------|------------------------------------|-------------------|--------------------|
| | | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Ethylamine | 1.26E+00 | g | 2.53E-03 | 2.71E-01 | 5.31E-03 | 1.43E-02 |
| ZSM-5 (Zeolita Socony Mobil – 5) | 8.86E-01 | g | | | 4.43E-02 | |
| Ethyl acetate (10 mL) | 2.62E+00 | g | 5.23E-03 | 3.31E+00 | 2.53E-01 | 6.82E-01 |
| Heating steam | 2.00E-03 | MJ | | | | |
| Electricity | 3.33E-04 | kWh | | | | |
| Chemical factory | 4.00E-13 | unit | | | | |
| Transport lorry>16t | 1.00E-04 | tkm | | | | |
| Transport train | 6.00E-04 | tkm | | | | |

Table 16. Ru₂Cl₄(CO)₆

| Inputs | Quantity for 1 g of product ¹⁰ | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------|---|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| RuCl ₃ | 8.51E-01 g | | | 4.09E-02 | |
| CO | 3.44E-01 g | 1.59E-02 | | | |
| 2-metoxietanol | 2.32E-01 g | 4.64E-04 | 2.55E-01 | 2.25E-02 | 6.05E-02 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

Table 17. N-(2-bromophenyl)benzamide

| Inputs | Quantity for 1 g of product ¹¹ | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------|---|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Benzoyl fluoride | 4.73E-01 g | | 3.73E-02 | 2.29E-03 | 6.17E-03 |
| 2-bromoaniline | 6.56E-01 g | | 3.19E-02 | 3.18E-03 | 8.55E-03 |
| Chlorobenzene | 3.21E+00 g | | 4.78E+00 | 3.11E-01 | 8.38E-01 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

Table 18. Copper Oxide (CuO) Nanoparticles

| Inputs | Quantity for 1 g of product ¹² | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------|---|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| CuSO ₄ | 2.11E+00 g | | | 2.46E-02 | 2.93E-02 |
| Citric acid | 2.55E+00 g | | 1.15E-01 | 1.28E-02 | 3.44E-02 |
| Deionized water | 5.09E+01 g | 1.02E-01 | | 4.58E+01 | 0.00E+00 |
| Ethylene glycol | 3.00E+00 g | 6.00E-03 | 1.21E+00 | 2.90E-01 | 7.82E-01 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

Table 19. Schiff base

| Inputs | Quantity for 1 g of product ⁵ | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|-----------------------------|--|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Salicylaldehyde (20.0 mmol) | 6.03E-01 g | | 5.56E-02 | 2.95E-03 | 7.93E-03 |
| o-aminophenol (30.0 mmol) | 8.08E-01 g | | 1.76E-01 | 2.88E-02 | 7.75E-02 |
| Methanol (10 mL) | 5.66E-01 g | 1.13E-03 | 4.94E-01 | 5.48E-02 | 1.48E-01 |
| Ice-cold methanol (5 mL) | 2.83E-01 g | 5.66E-04 | 2.47E-01 | 2.74E-02 | 7.38E-02 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

Table 20. Silica supported PCC

| Inputs | Quantity for 1 g of product ⁶ | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|-------------------------------|--|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| Silica gel 100-200 mesh | 4.68E+00 g | | | 1.17E-02 | 8.82E-02 |
| Pyridine-chlorochromate (PCC) | 1.05E+00 g | | 4.09E-02 | 5.11E-03 | 1.37E-02 |
| Acetone (200 mL) | 1.07E+00 g | 2.15E-03 | 1.55E+00 | 1.04E-01 | 2.80E-01 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

Table 21. Pyridine-chlorochromate (PCC)

| Inputs | Quantity for 1 g of product ¹³ | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|---------------------|---|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| CrO ₃ | 5.53E-01 g | | | 4.46E-02 | 4.46E-02 |
| HCl | 2.22E-01 g | | | 5.25E-02 | |
| Pyridine | 4.38E-01 g | 8.75E-04 | 1.23E-01 | 6.76E-03 | 1.82E-02 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

Table 22. Benzo[d]oxazole

| Inputs | Quantity for 1 g of product ⁷ | Process air emissions (g) | Wastewater treatment emissions (g) | | |
|--------------------------------|--|---------------------------|------------------------------------|-------------------|--------------------|
| | | | CO ₂ to air | Compound to river | Sludge to landfill |
| N-(2-bromophenyl)formamide | 1.77E+00 g | | 8.64E-02 | 8.57E-03 | 2.31E-02 |
| CuO | 4.00E-02 g | | | 1.00E-02 | 1.19E-02 |
| K ₂ CO ₃ | 2.00E+00 g | 4.00E-03 | | 2.00E+00 | 0.00E+00 |
| Heating steam | 2.00E-03 MJ | | | | |
| Electricity | 3.33E-04 kWh | | | | |
| Chemical factory | 4.00E-13 unit | | | | |
| Transport lorry>16t | 1.00E-04 tkm | | | | |
| Transport train | 6.00E-04 tkm | | | | |

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