Prospective inventory modelling of emerging chemicals: The case of photonic materials

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1. Introduction

Prospective life cycle assessment (LCA), or ex-ante LCA, has been defined as an assessment of a product system modeled at a future time, before its commercialization [1]. Such assessments bring the promise of altering emerging technologies in a more environmentally benefitial direction before they become difficult to change. Since the future cannot be known with certainty, prospective modeling need to rely on scenarios of various kinds. However, how to conduct such prospective scenario modeling in practice still has to be clarified. Photon upconversion is a technology aimed at converting low-energy light into higher-energy light harvestable by solar photovoltaics, thereby increasing their efficiency [2]. Two low-energy photons are captured and converted into a single high-energy photon. In order to do that, current research suggest that two photonic materials are needed: a sensitizer molecule that converts photons to an excited state and an annihilator molecule that combines these excited states into a single high-energy photon. Two chemicals currently considered for sensitizers and annihilators are ruthenium bipyridine chloride (RBC) and diphenylanthracene (DPA), respectivly (Figure 1). These novel, emerging chemicals have not been studied regarding environmental performance before and are consequently not present in any LCA databases. The aim of this study is to present a generic procedure for prospective inventory modeling of emerging chemicals and apply that to the cases of RBC and DPA by developing unit processes for these two chemicals.

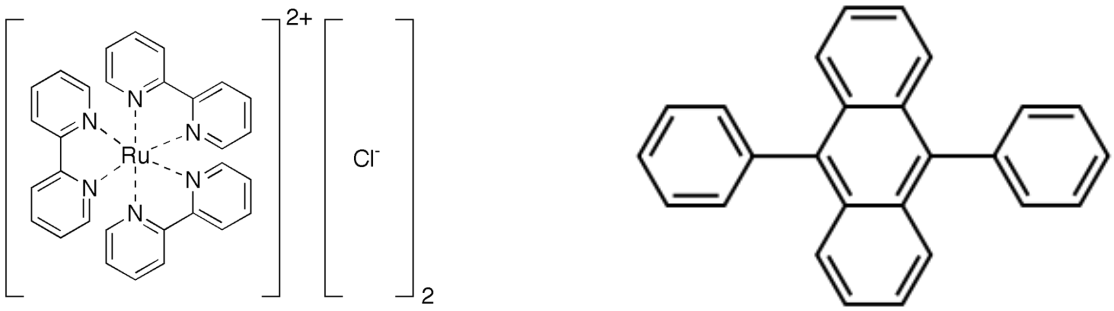

Figure 1: Chemical structures of ruthenium bipyridine chloride (RBC, left) and diphenylanthracene (DPA, right).

2. Materials and methods

An industrial synthesis scenario was adopted as our main scenario, reflecting a possible future time when RBC and DPA are produced at an industrials cale. The modeling was conducted in six steps. First, likely syntheses were identified. RBC ($[Ru(bby)_3]Cl_2$) requires two inputs: bipyridine (bpy) and ruthenium chloride ($RuCl_3$):

$$3(bpy) + RuCl_3 \rightarrow [Ru(bpy)_3]Cl_2$$

DPA requires three inputs: anthraquinone ($C_{14}H_8O_2$), phenyllithium (C_6H_5Li) and toluene as solvent. A by-product of this synthesis is lithium oxide (Li_2O):

$$C_{14}H_8O_2 + 2C_6H_5Li \rightarrow C_{26}H_{18} + Li_2O$$

Second, inputs and outputs were calculated stoichiometrically based on the two reactions above. Third, yields were obtained to modify the stoichiometric inputs and outputs to reflect reasonable future industry practice. For RBC, patent data suggest that the yield is 60% for bipyridine and 100% for $RuCl_3$ due to effective recovery. Based on generic industrial reaction yields, 90% was assumed for DPA synthesis. Patent data suggest a 20:1 molar ratio for toluene:DPA. A 95% toluene solvent recovery with associated inputs was assumed based on ref. [3]. Fourth, outputs were categorized as by-products or waste. Lithium oxide was

considered a by-product since it has important industrial uses. Since there is no industrial use for unrecovered toluene, it was considered liquid waste. Fifth, emissions were estimated. In this case, only toluene is considered volatile and toxic enough to be a concern, for which emissions were estimated using a generic industrial-scale emission factor [3]. Sixth, energy flows were modeled. Since the syntheses are conducted at room temperature and 50°C, respectively, heating energy was considered negligible.

3. Results and discussion

The unit processes for RBC and DPA can be found in Tables 1 and 2, respectivley. As can be seen, unit processes can be developed following this generic procedure. In particular inputs are well-captured by this modeling approach, since they largely originate from stochiometric chemical reactions. Outputs are captured relatively well, since they too can largely be obtained from chemical reactions. However, the use of solvents, catalysts and similar non-stoichiometric inputs might not be captured as well. Emissions and energy flows, which are not obtained from the chemical reactions, are captured less well. For syntheses involving high temperatures, energy requirements cannot be assumed negligible as in this case, but need to be modeled.

Material	Type	Quantity	Unit
Ruthenium bipyridine chloride	Main product	1	kg
Bipyridine	Input	1.2	kg
Ruthenium chloride	Input	0.32	kg

Table 1: Unit process for production of ruthenium bipyridine chloride.

Material	Type	Quantity	Unit
Diphenylanthracene	Main product	1	kg
Anthraquinone	Input	0.70	kg
Phenyllithium	Input	0.57	kg
Toluene	Input	0.28	kg
Steam	Input	7.9	kg
Electricity	Input	1.1	MJ
Water	Input	420	kg
Nitrogen gas	Input	0.053	Nm^3
Lithium oxide	By-product	0.081	kg
Toluene	Waste	0.28	kg
Toluene	Emission	5.6×10^{-7}	kg

Table 2: Unit process for production of diphenylanthracene.

4. Conclusions

We propose the following generic procedure for unit-process modeling of emerging chemicals:

1. Identify likely chemical syntheses.
2. Calculate inputs stoichiometrically.
3. Modify inputs based on available yields for reactants and solvents (e.g. obtained from patents or estimated).
4. Categorize outputs as by-products or waste.
5. Calculate process emissions.
6. Model energy flows.

Further research into the modeling of energy flows for high-temperature processes is recommended, as well as estimation procedures for emissions from emerging chemicals production.

5. References

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