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# STUDY OF THE SYNTHESIS OF ZERO-VALENT IRON NANOPARTICLES THROUGH LIFE CYCLE ASSESSMENT


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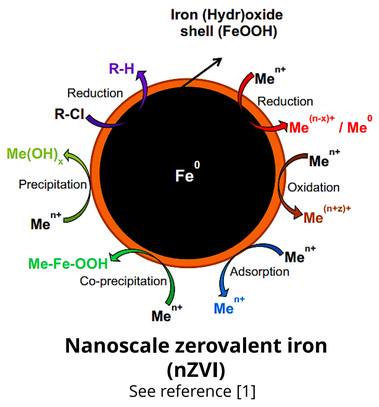
## INTRODUCTION




**Nanoscale zerovalent iron (nZVI)**
See reference [1]

### Synthesis methods

- Traditional chemical method: reduction of Fe(II) or Fe(III) using sodium borohydride. [3]
- Reduction of goethite or hematite using hydrogen.
- "Green" methods: using polyphenols.
- "Semi-green" methods: using sodium dithionite and borohydride.
- Milling (top-down)

The morphology, composition, and reactivity of nZVI vary based on the chosen synthesis method. [2]
In this work, the traditional method will be considered for protocols S2015 and S2023.

### Life Cycle Assessment (LCA)

An environmental management technique standardized by ISO 14040 and ISO 14044. It has the potential to identify critical stages, enabling the reduction of environmental impacts in both production and remediation processes. [4]

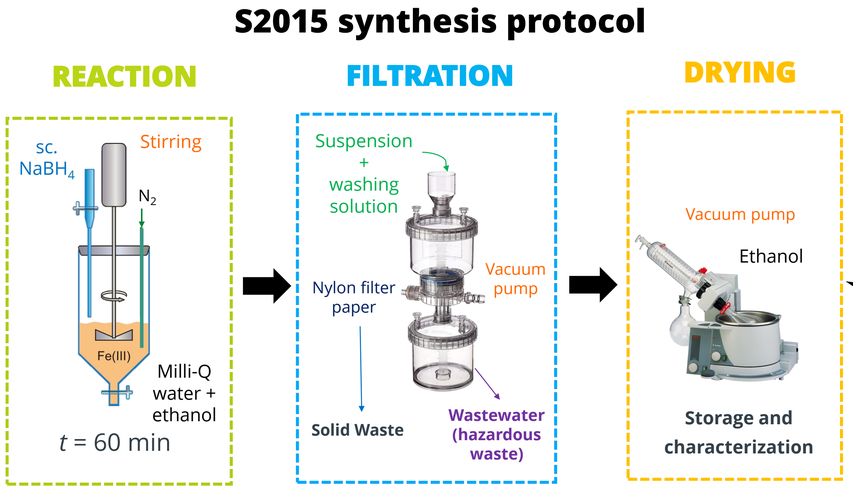
### Objetive

To compare two laboratory-tested synthesis protocols for producing nZVI, based on the traditional method, through the application of LCA.

**S2023 vs S2015**

## MATERIALS AND METHODS

### S2015 synthesis protocol




### Changes introduced by S2023

**Reaction stage**
- ✓ A syringe pump was added.
- ✓ The reaction time was reduced to 30 minutes.
- ✓ The 40% ethanol solution was replaced with absolute ethanol.

**Filtration stage**
- ✓ The washing solution was reduced, using only absolute ethanol.

**Drying stage**
- ✓ The rotary evaporator was replaced with a vacuum desiccator.

### Characterization results

| Results | S2015 | S2023 |
|---|---|---|
| Fe(0) (g/100 g nZVI) | 58 | **87** ✓ |
| nZVI mass produced (g) | 0,22 | **0,38** ✓ |
| Size (nm) | **10 – 60** ✓ | 50 – 103 |

### LCA

**Step 1: Define**

- ✓ **Scope:** Cradle to gate
- ✓ **Funtional unit:** 1 g of nZVI produced

## RESULTS

### Step 2: Inventory

Based on the synthesis data, the inventory was constructed using 1 g of nZVI as a functional unit.

| Inventory | S2015 | S2023 |
|---|---|---|
| **INPUTS** | | |
| $FeCl_3$ (kg) | $5.91 \times 10^{-3}$ | $3.42 \times 10^{-3}$ |
| $NaBH_4$ (kg) | $2.97 \times 10^{-3}$ | $1.71 \times 10^{-3}$ |
| Ethanol (kg) | $4.60 \times 10^{-1}$ | $4.58 \times 10^{-1}$ |
| NaOH (kg) | $3.27 \times 10^{-4}$ | Not used |
| Milli-Q water (kg) | $6.00 \times 10^{-1}$ | Not used |
| $N_2$ gas (kg) | **$1.62 \times 10^{-1}$** | $8.01 \times 10^{-2}$ |
| Filter paper (kg) | $1.13 \times 10^{-2}$ | $1.13 \times 10^{-2}$ |
| **Energy** | **3.20** | 0.76 |
| Stirring (kWh) | $3.41 \times 10^{-2}$ | $2.44 \times 10^{-2}$ |
| Filtration (kWh) | $1.41 \times 10^{-1}$ | $4.91 \times 10^{-1}$ |
| Drying (kWh) | **3.02** | $2.45 \times 10^{-1}$ |
| **OUTPUTS** | | |
| Solid waste (kg) | $1.13 \times 10^{-2}$ | $1.13 \times 10^{-2}$ |
| Wastewater (kg) | $7.81 \times 10^{-1}$ | $4.62 \times 10^{-1}$ |
| nZVI (kg) | 0.001 | 0.001 |

The quantities used in both cases are of the same order.

- ✓ In S2023, NaOH is not used to adjust the pH.
- ✓ In S2015, drying energy is significant.

### Step 3: Life Cycle Impact Assessment

For the analysis, the process was divided into four stages.

- Effluents
- Drying
- Filtration
- Reaction

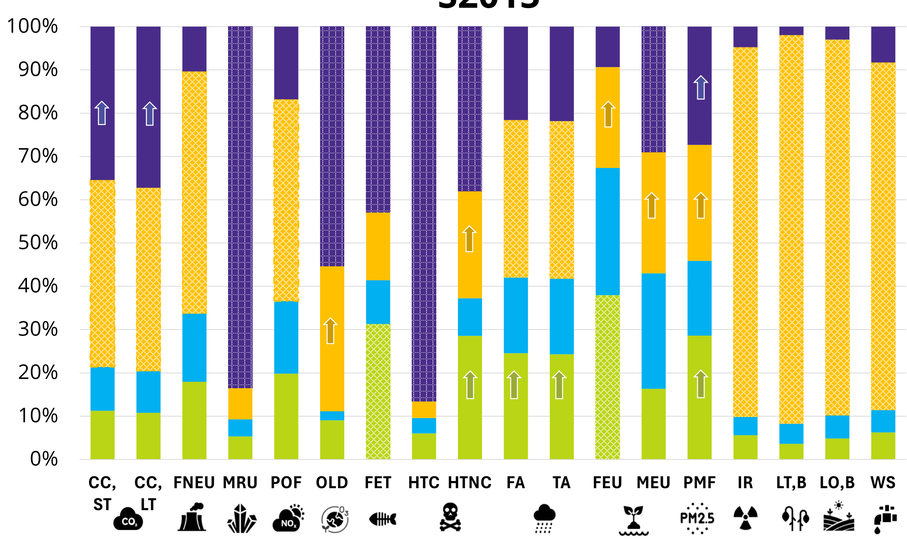
For the impact analysis,
- SimaPro® v9.5
- Ecoinvent 3.9.1
- IMPACT World+ (Midpoint V1.03)

were used.

With the results, 100% stacked column charts were created, and the impacts of each stage were plotted for 18 impact categories

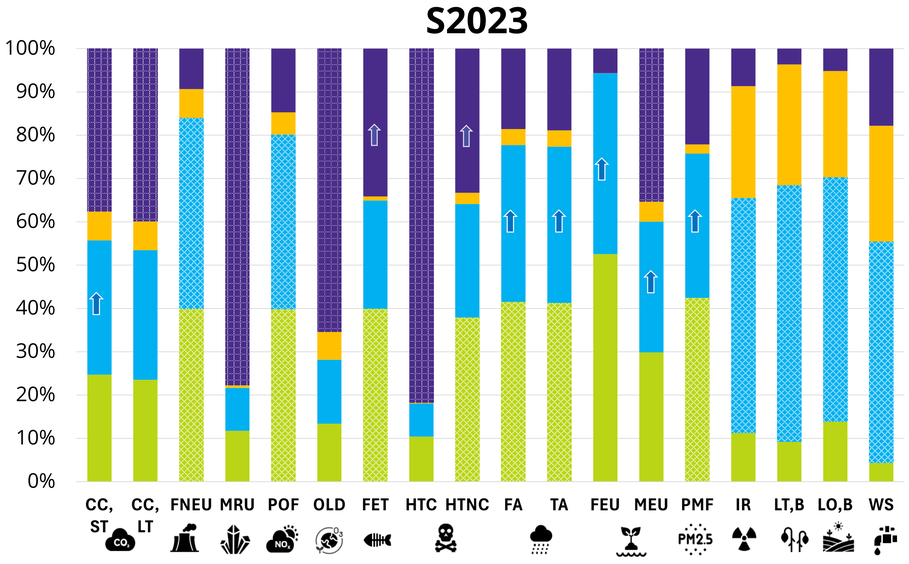
*CC, ST: Climate change, short term / CC, LT: CC, long term / FNEU: Fossil and nuclear energy use / MRU: Mineral resources use / POF: Photochemical oxidant formation / OLD: Ozone layer depletion / FET: Freshwater ecotoxicity / HMC: Human toxicity cancer / HTNC: HT non-cancer / FA: Freshwater acidification / TA: Terrestrial acidification / FEU: Freshwater eutrophication / MEU: Marine eutrophication / PMF: Particulate matter formation / IR: Ionizing radiation / LT,B: Land transformation, biodiversity / LO,B: Land occupation, biodiversity / WS: Water scarcity*

**S2015**




Stages with highest contribution
- ✓ Drying: **10** categories (5)
- ✓ Effluents: **6** categories (3)
- ✓ Reaction: **2** categories (4)

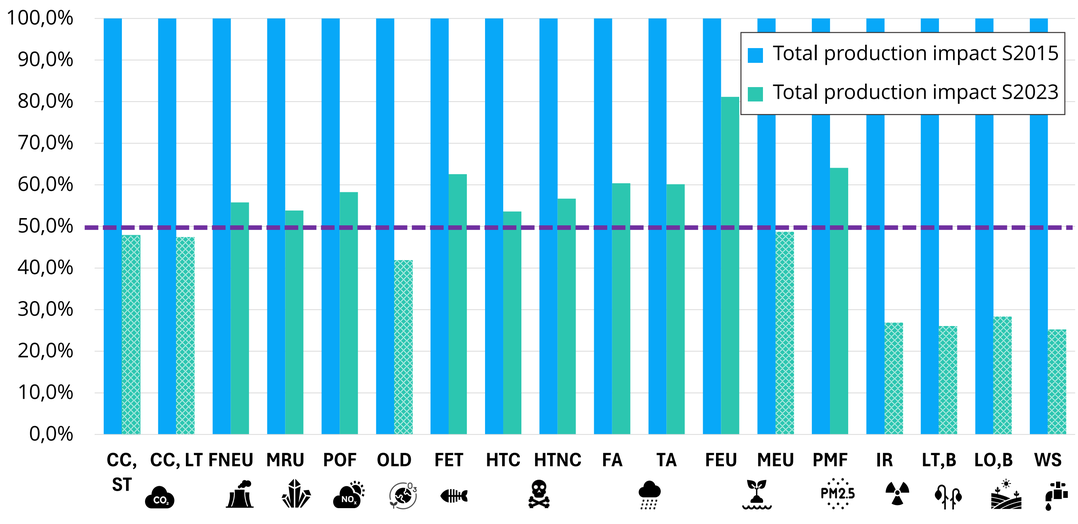
**S2023**




Stages with highest contribution
- ✓ Reaction: **8** categories
- ✓ Effluents: **6** categories (2)
- ✓ Filtration: **6** categories (6)

**Note:** The numbers in parentheses represent other relevant categories for each stage. Although they are not the main contributors, they highlight notable secondary effects to consider in the analysis.

### S2015 vs S2023




To compare both methods, the impact values were normalized relative to S2015, revealing:

- ✓ A significant reduction in all categories for S2023.
- ✓ Reduction of more than 50% of the absolute value in 8 categories

## CONCLUSIONS

1. The S2023 protocol led to an improvement in nZVI production:
   - ➢ Increased synthesized nZVI mass.
   - ➢ Increased %Fe(0).
2. Vacuum drying using a desiccator significantly reduced environmental impacts across all impact categories.
3. Filtration and effluent disposal are the critical stages in the new method.
4. A suggested next step is to apply a cradle-to-use approach, including the remediation stage in the functional unit.

## REFERENCES


[1] O'Carrol (2013)
[2] Kharisov (2012)
[3] Zhang (2003)
[4] Quici, Crespi, Montesinos (2024)