

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

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INTRODUCTION



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.



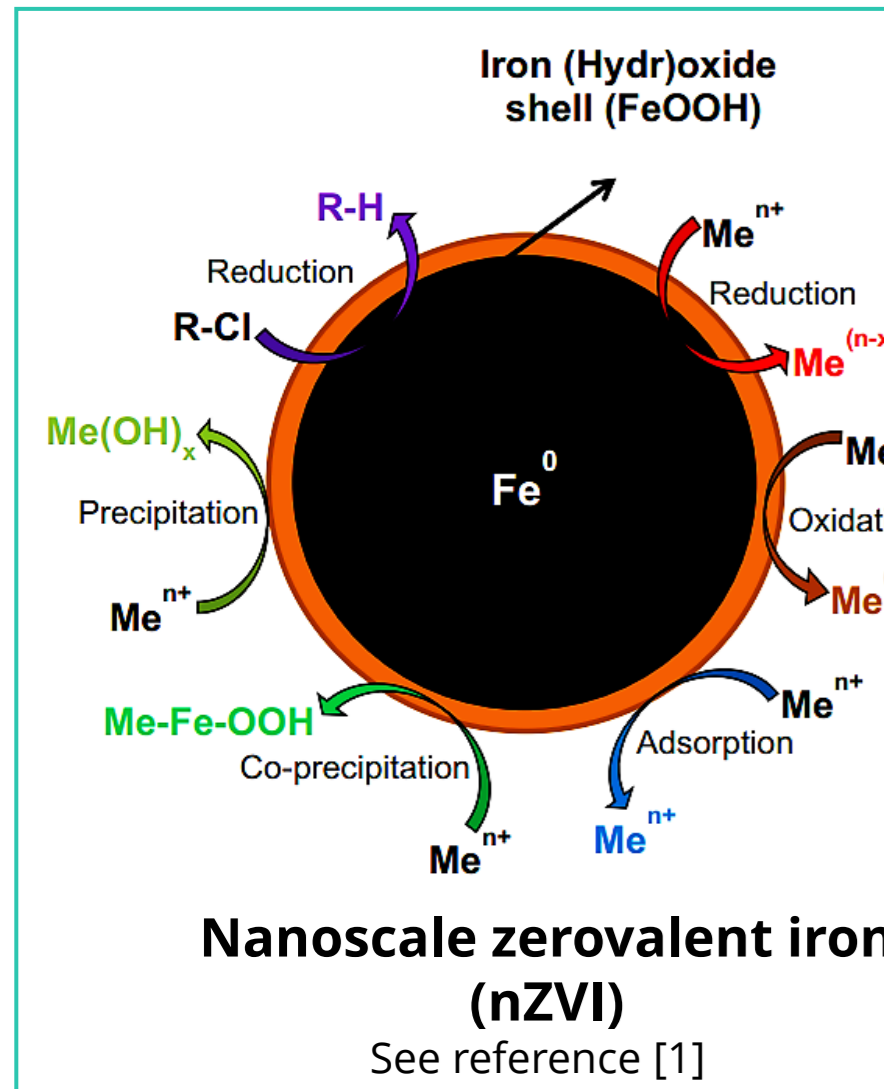
Life Cycle Assessment (LCA)

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]

Objective

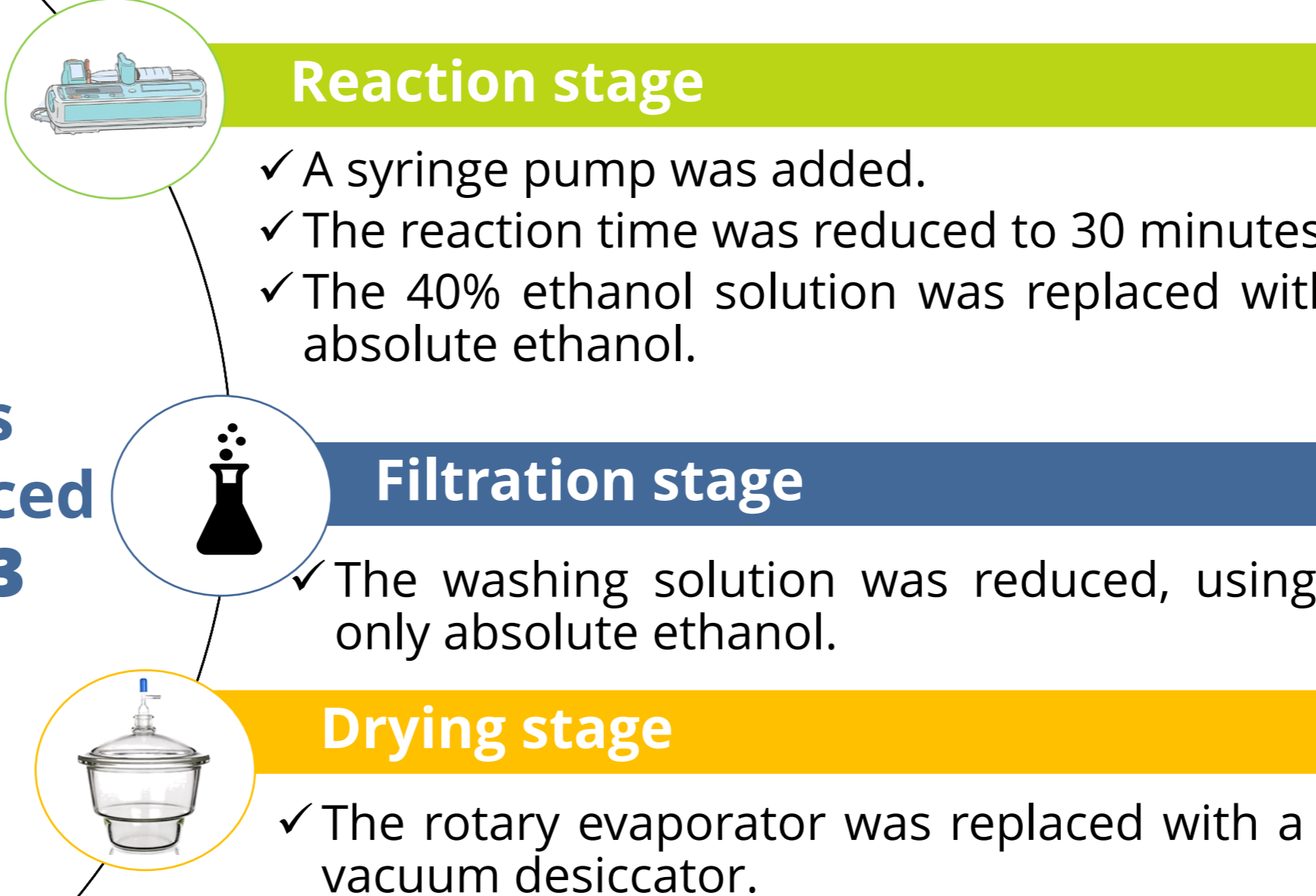
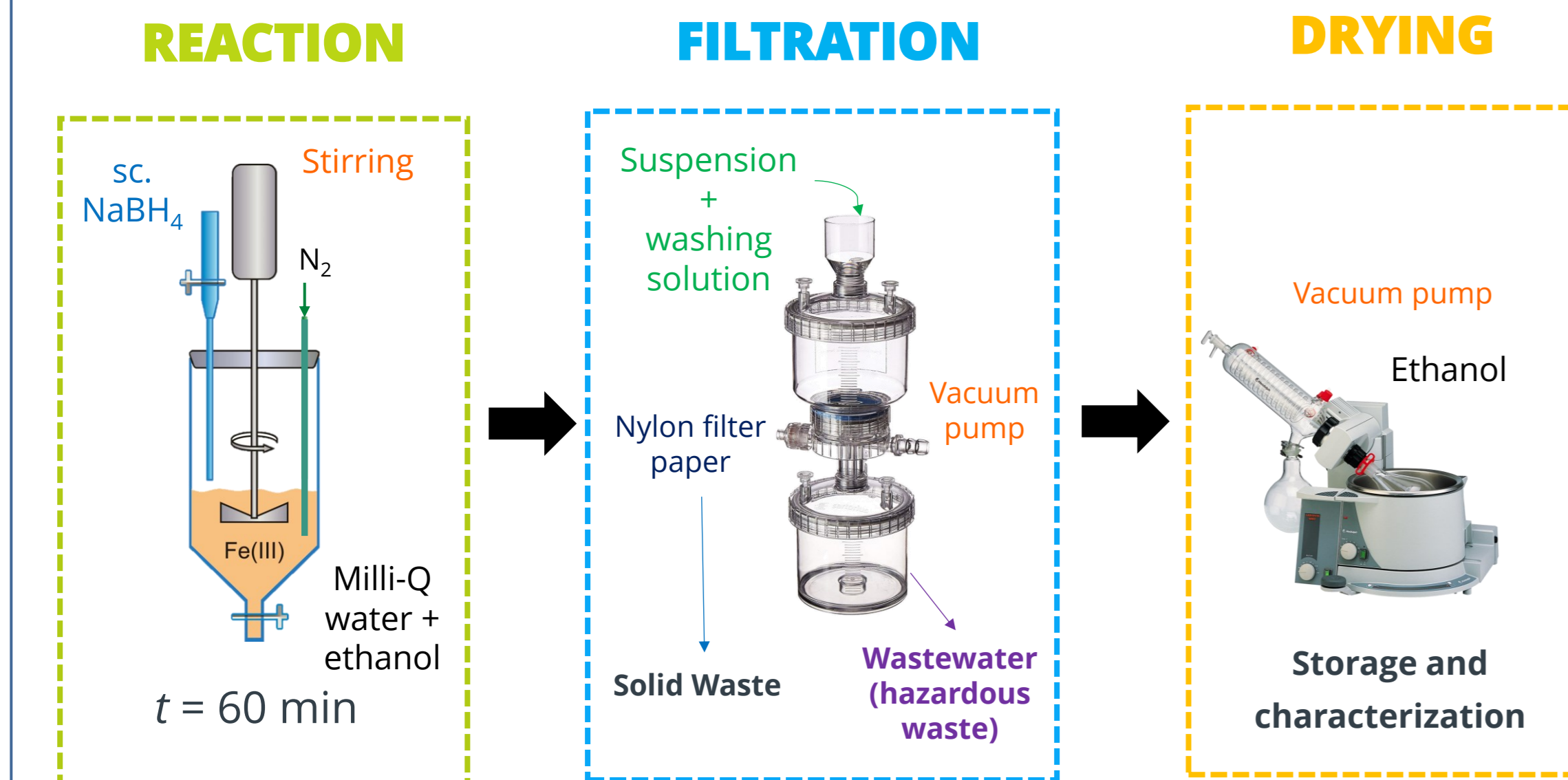
To compare two laboratory-tested synthesis protocols for producing nZVI, based on the traditional method, through the application of LCA.

S2023 vs S2015



MATERIALS AND METHODS

S2015 synthesis protocol



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
✓ **Functional 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 × 10 ⁻³	3.42 × 10 ⁻³
NaBH ₄ (kg)	2.97 × 10 ⁻³	1.71 × 10 ⁻³
Ethanol (kg)	4.60 × 10 ⁻¹	4.58 × 10 ⁻¹
NaOH (kg)	3.27 × 10 ⁻⁴	Not used
Milli-Q water (kg)	6.00 × 10 ⁻¹	Not used
N ₂ gas (kg)	1.62 × 10 ⁻¹	8.01 × 10 ⁻²
Filter paper (kg)	1.13 × 10 ⁻²	1.13 × 10 ⁻²
Energy	3.20	0.76
Stirring (kWh)	3.41 × 10 ⁻²	2.44 × 10 ⁻²
Filtration (kWh)	1.41 × 10 ⁻¹	4.91 × 10 ⁻¹
Drying (kWh)	3.02	2.45 × 10 ⁻¹
OUTPUTS		
Solid waste (kg)	1.13 × 10 ⁻²	1.13 × 10 ⁻²
Wastewater (kg)	7.81 × 10 ⁻¹	4.62 × 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.

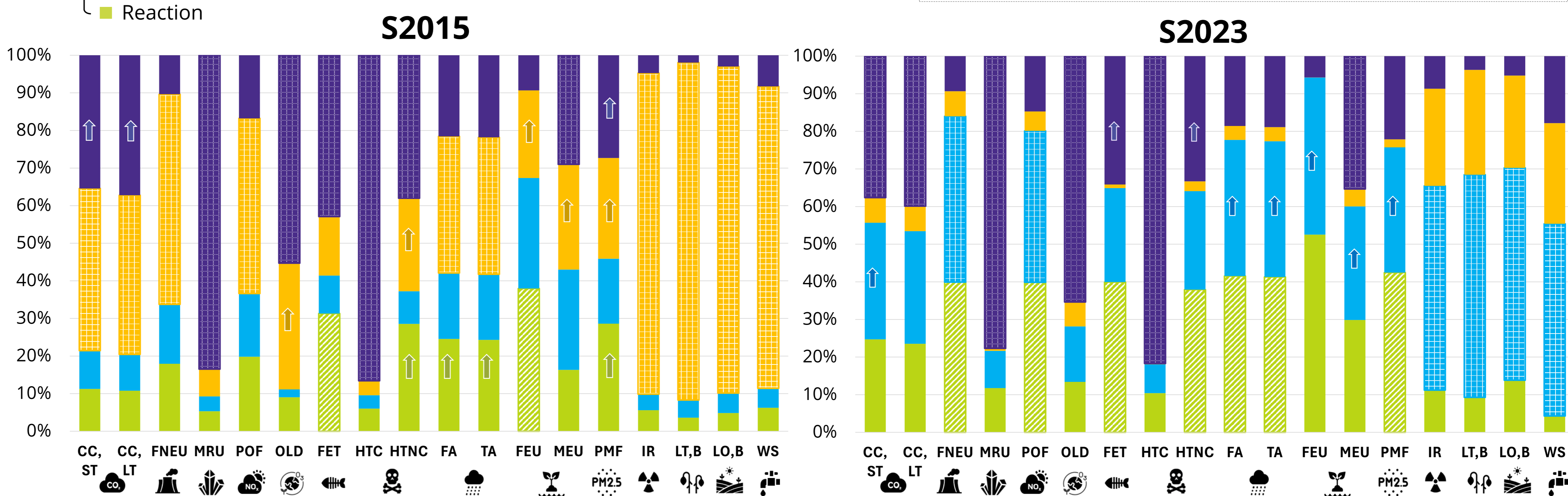
Step 3: Life Cycle Impact Assessment

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

For the impact analysis, SimaPro® v9.5, Ecoinvent 3.9.1, and 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

- Effluents
- Drying
- Filtration
- Reaction

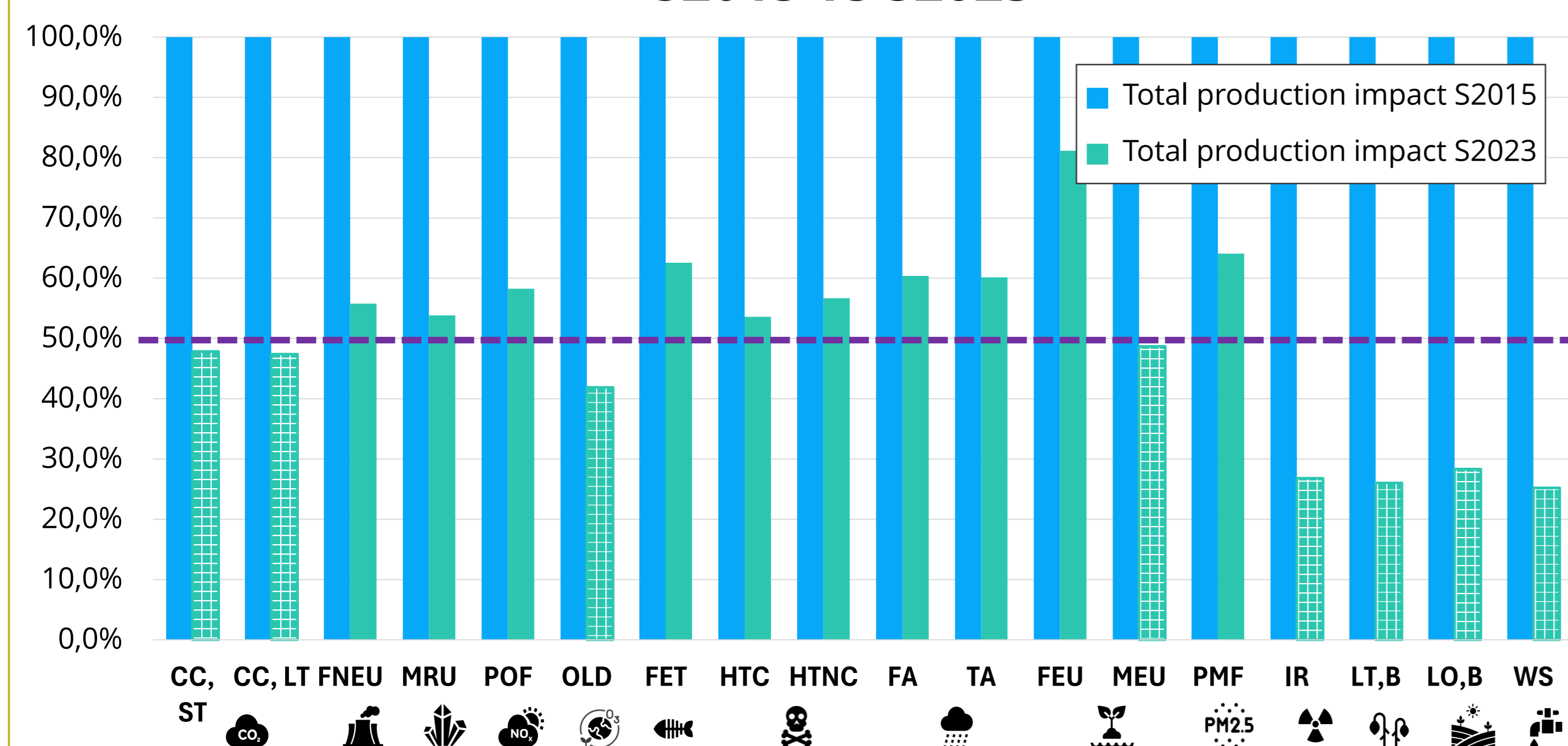


Stages with highest contribution
 ✓ Drying: 10 categories (5)
 ✓ Reaction: 2 categories (4)

Stages with highest contribution
 ✓ Reaction: 8 categories
 ✓ 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

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

REFERENCES

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