ZEOCAT-3D

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 814548

ZEOCAT – 3D:

OVERVIEW AND MAIN GOALS

María Tripiana Serrano

Basic project data

Title	Development of a bifunctional hierarchically structured zeolite based nano-catalyst using 3D-technology for direct conversion of methane into aromatic hydrocarbons via methane dehydroaromatization
Acronym	ZEOCAT-3D
Grant Agreement number	814548
Coordinator	OPTIMIZACION ORIENTADA A LA SOSTENIBILIDAD SL (IDENER)
Start date	1st of April 2019
End date	30th of September 2022
Overall Budget	€ 6,764,020
Eu Contribution	€ 6,764,020
Call	H2020-NMBP-ST-IND-2018
Topic	CE-NMBP-24-2018 - Catalytic transformation of hydrocarbons (RIA)

Table of contents

1 The context

The context

1

Aromatics are esential for some of the most extensive petrochemical products

2

Their utilization is associated with severe environmental consequences (aquatic species destruction, global warming,..)

3

Current production methods are cosidered usustainable

The context

1

Aromatics are esential for some of the most extensive petrochemical products

2

Their utilization is associated with severe environmental consequences (aquatic species destruction, global warming,..)

3

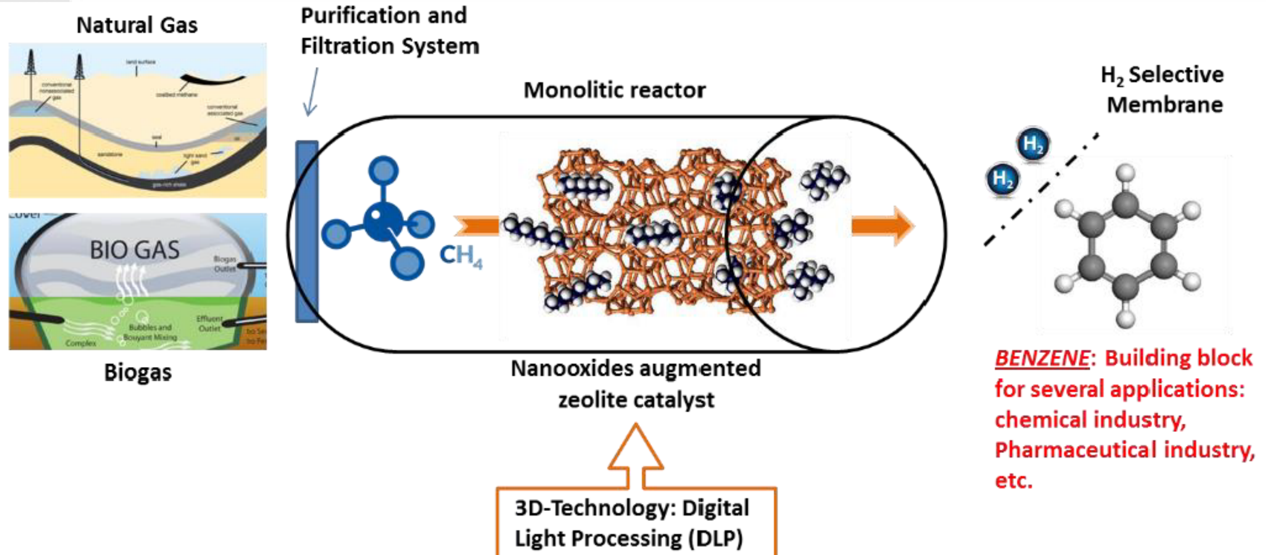
Current production methods are cosidered usustainable

The ZEOCAT-3D project proposes an alternative, which consists of obtaining these high-value chemicals (benzene, naphthalene, among others) from methane from sources like biogas and natural gas through an improved catalytic process called methane dehydroaromatization (MDA).

2 Main goal and objectives

Main goal and objectives

The goal of the project ZEOCAT-3D is the development of a new bi-functional (two types of active centers) structured catalysts, achieving for the first time a tetramodal pore size distribution (micro-, meso1-, meso2-, macro-porous) and high dispersion of metal active sites for the conversion of methane, coming from different sources as natural gas and biogas, into high value chemicals such as aromatics (benzene, naphthalene, among others) via methane dehydroaromatization (MDA).



Main goal and objectives

1 Development and production of an improved catalyst

2 Design, construction and validation of a catalytic reactor

3 Rational design of catalyst / Multiscale modelling

Main goal and objectives

1. Development and production of an improved catalyst

2. Design, construction and validation of a catalytic reactor

3. Rational design of catalyst / Multiscale modelling

→

- ✓ Improved methane conversion (>50%)
- ✓ Increased selectivity towards benzene (>90%)
- ✓ Enhanced performance (7 times less deactivation)
- ✓ Higher yield rates (up to 80%)

3 Challenges and solutions

Challenges and solutions

Challenges of the MDA process

Difficult activation of the C-H bond of CH_4 molecule, high reactivity of the products compared to methane, and acid sites of zeolites are occupied by coke deposition.

Problems to solve

The main drawbacks associated the process are low methane conversion, low selectivity towards the desired products and the quick deactivation due to carbon deposition onto the catalyst.

The solution

These problems will be overcome by the use of hierarchical zeolites structures synthesized by 3D-printing and loaded with doped molybdenum nano-oxides.

Challenges and solutions (Key elements)

ZEOCAT-3D

Catalyst

Development and production of improved catalyst, a 3D hierarchical structure with bi-functional activity (two types of active centers).

Reactor

Design, construction and validation of catalytic reactor, with improved productivity for direct methane MDA into aromatics.

Modelling

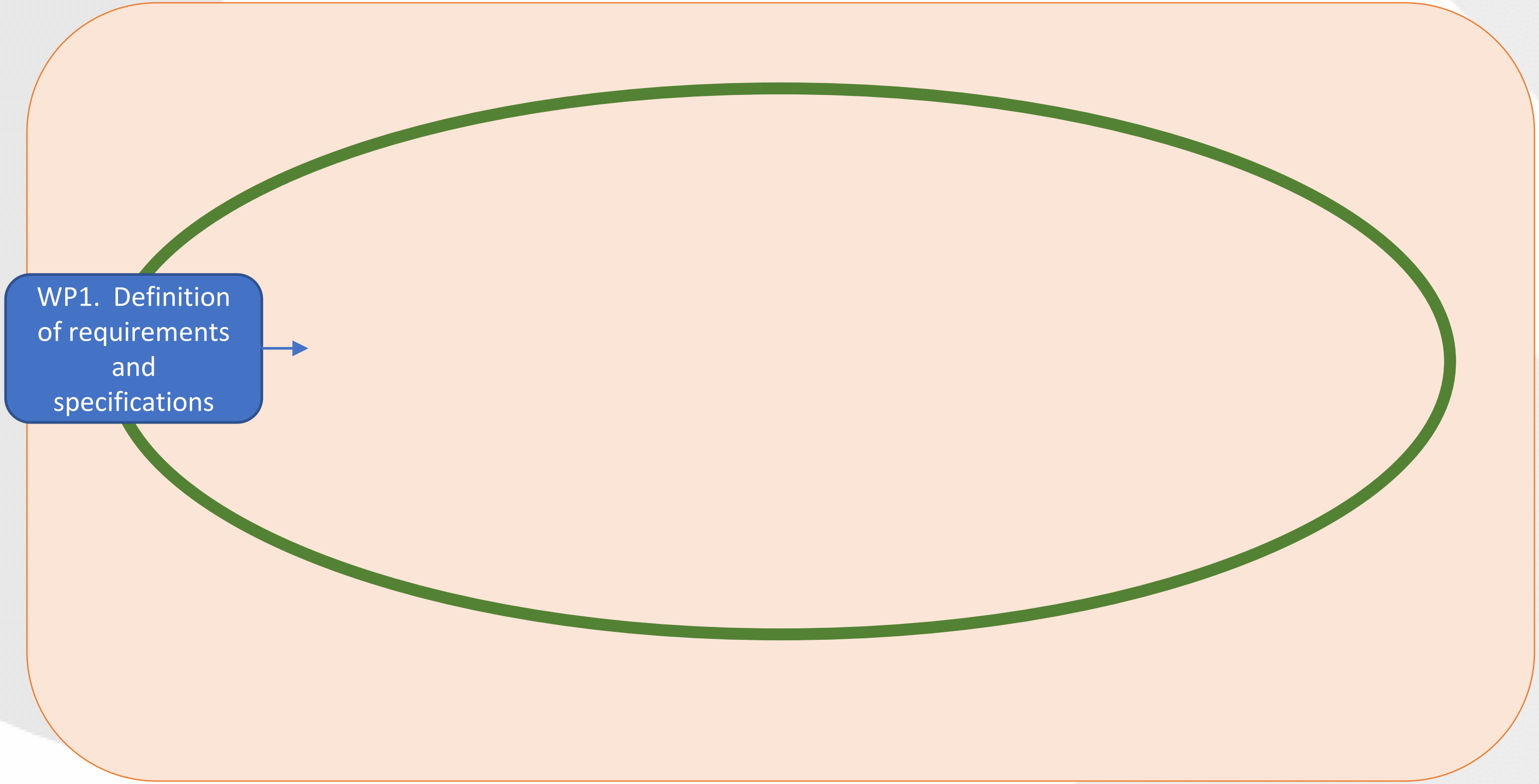
Rational design of catalyst/multi-scale modelling, for achieving multimodal pore size distribution (micro-, meso1-, meso2-, macro-porous).

Feedstock

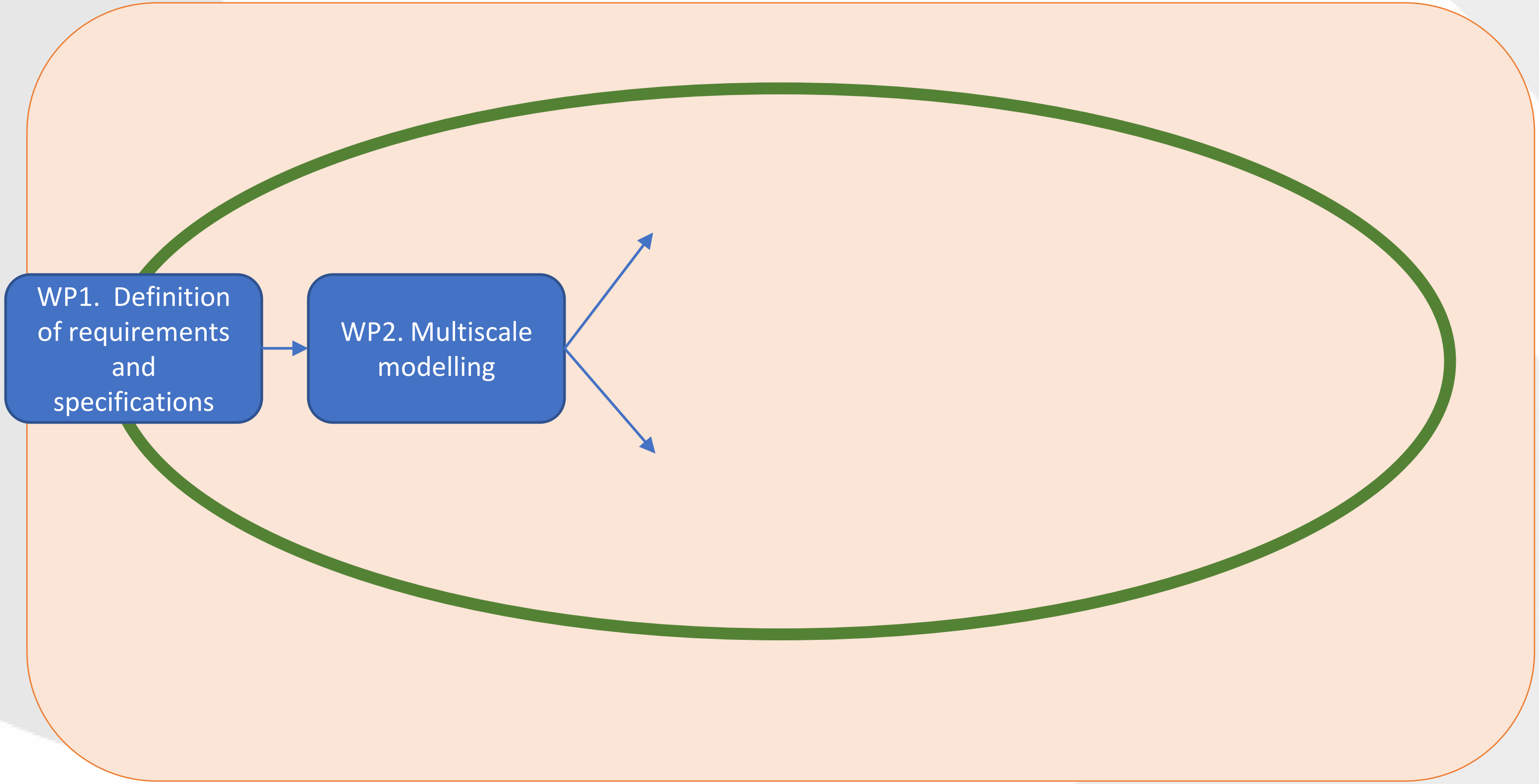
Optimization for different methane feedstock, which will bring enormous advantages for increasing the exploitation of natural gas and biogas.

4 Implementation

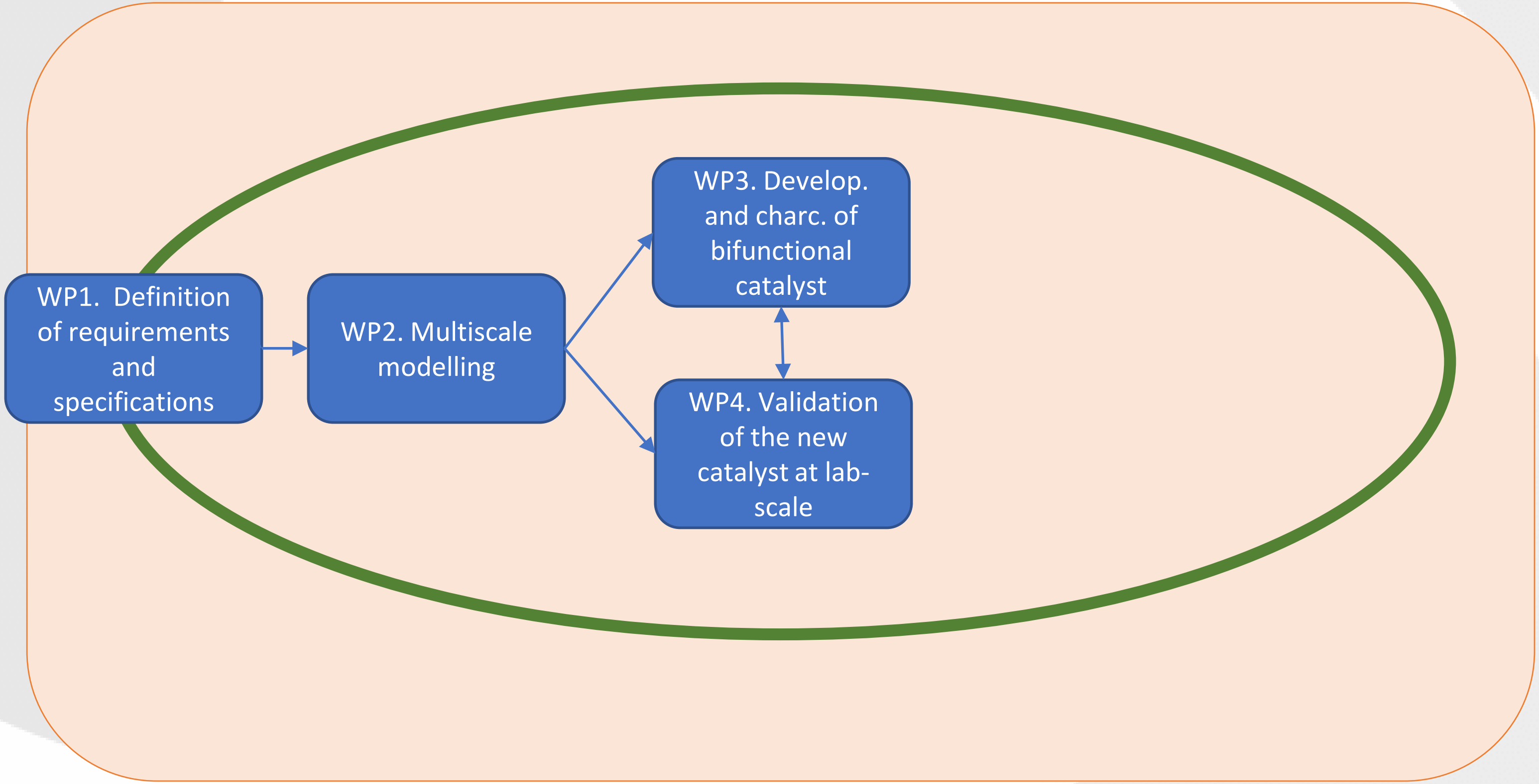
Implementation



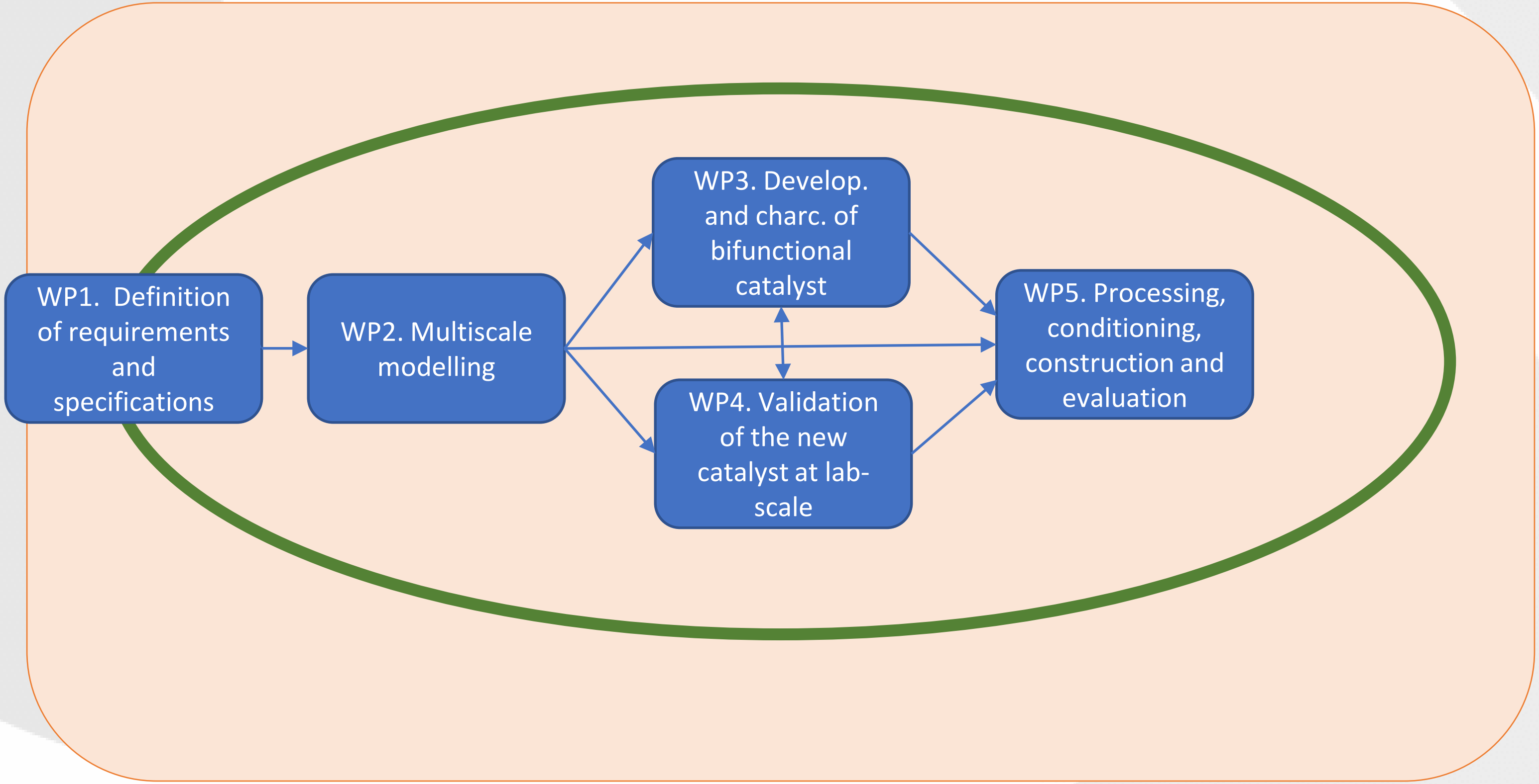
Implementation



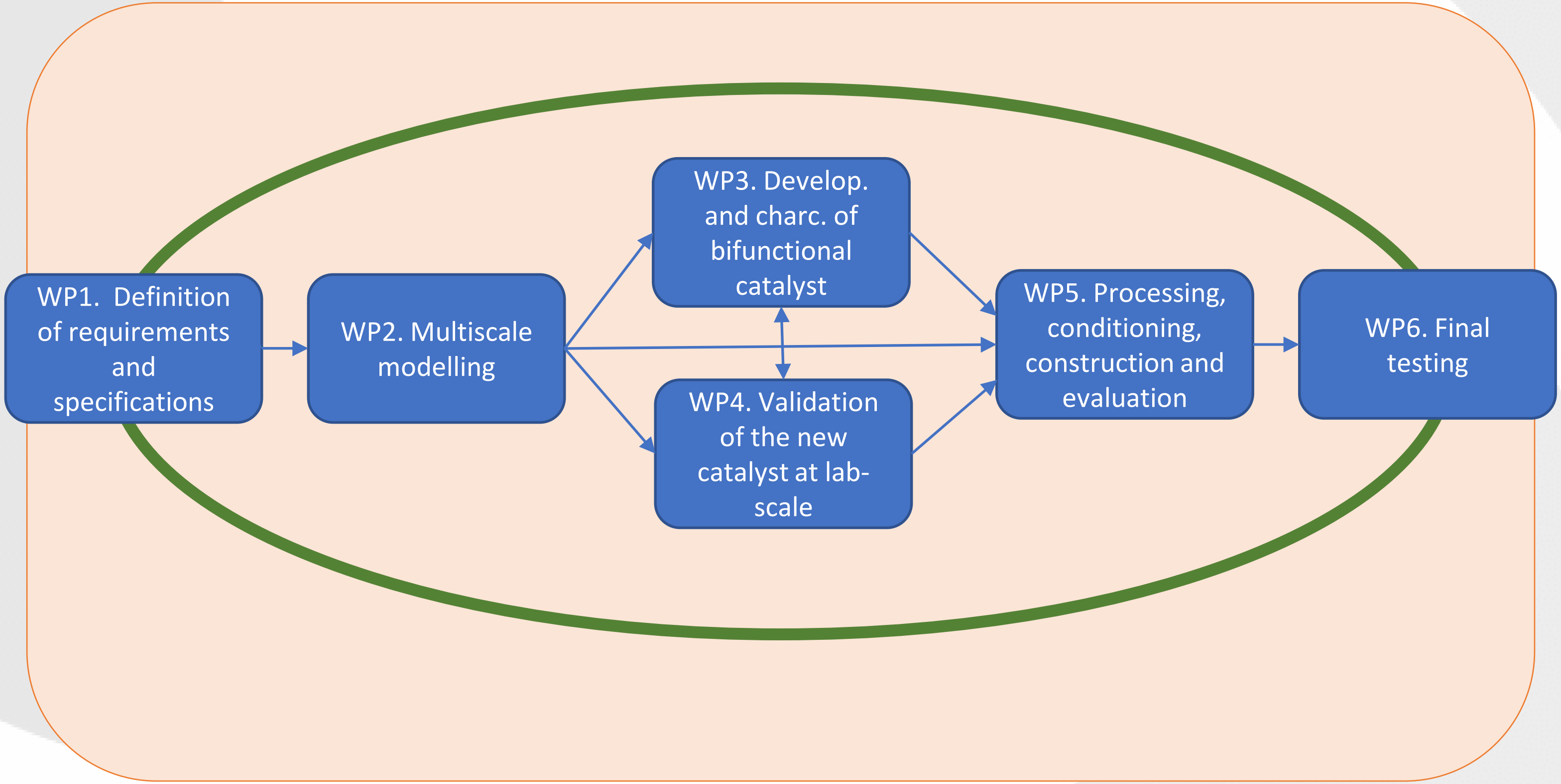
Implementation



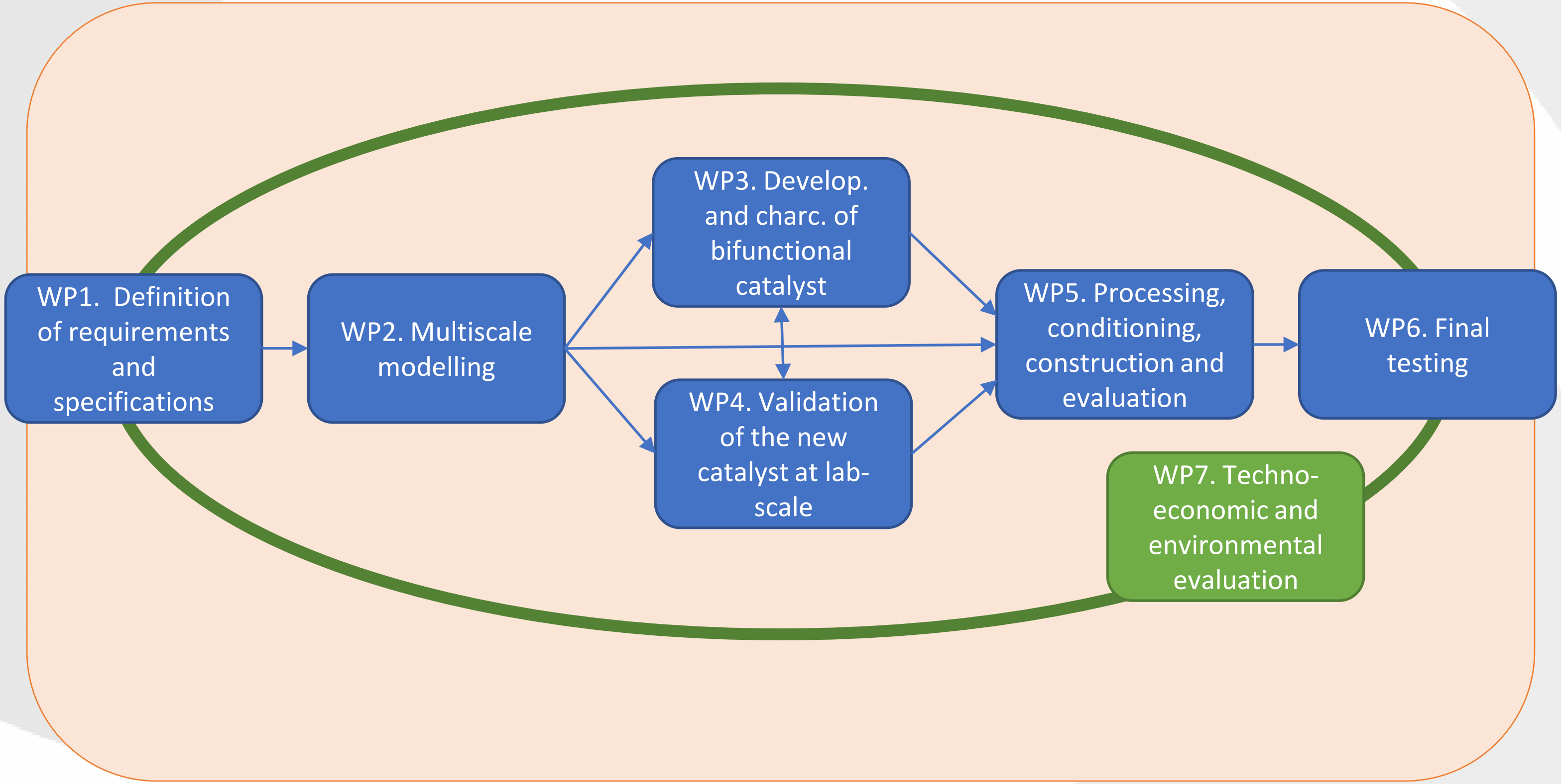
Implementation



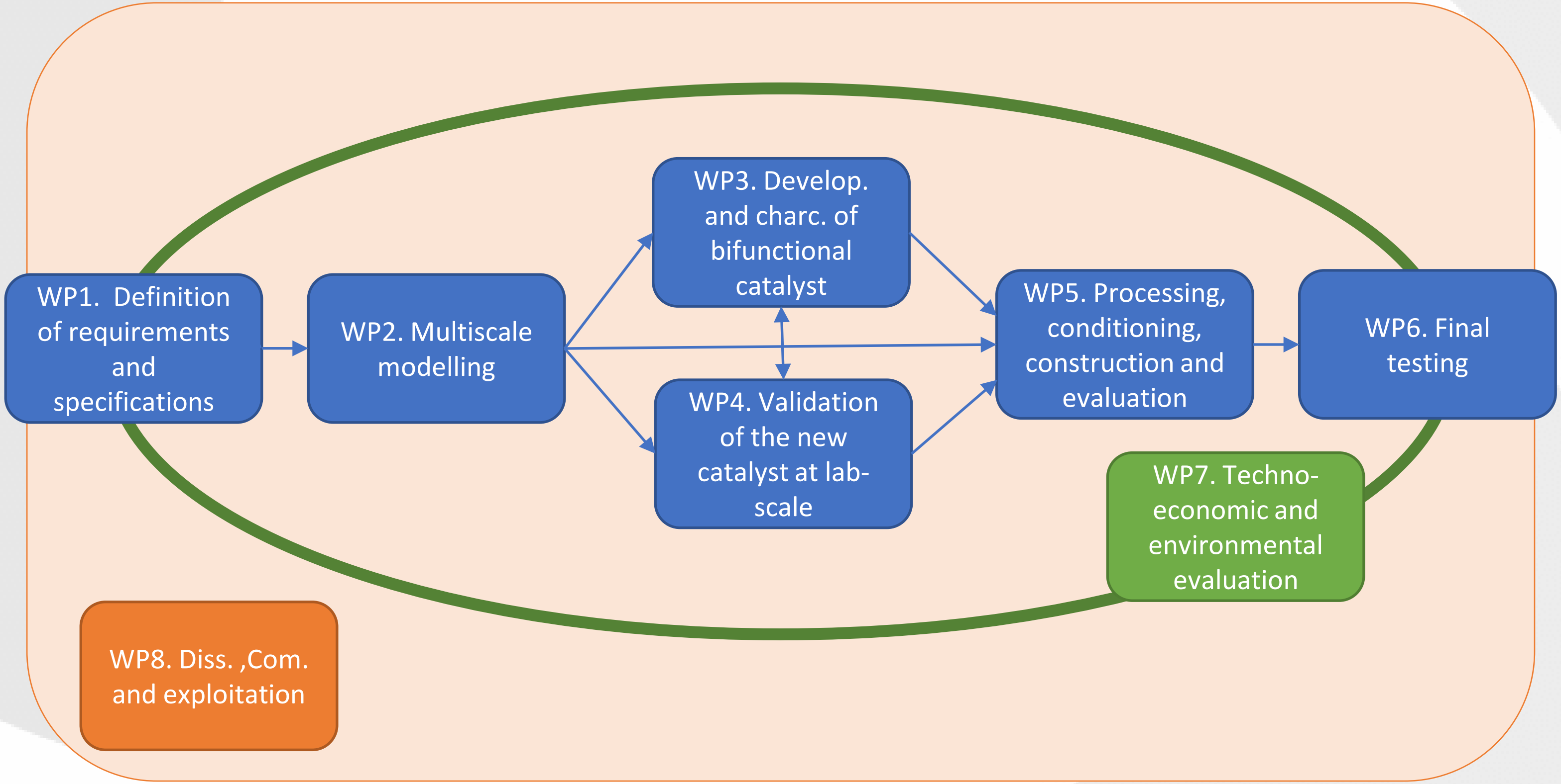
Implementation



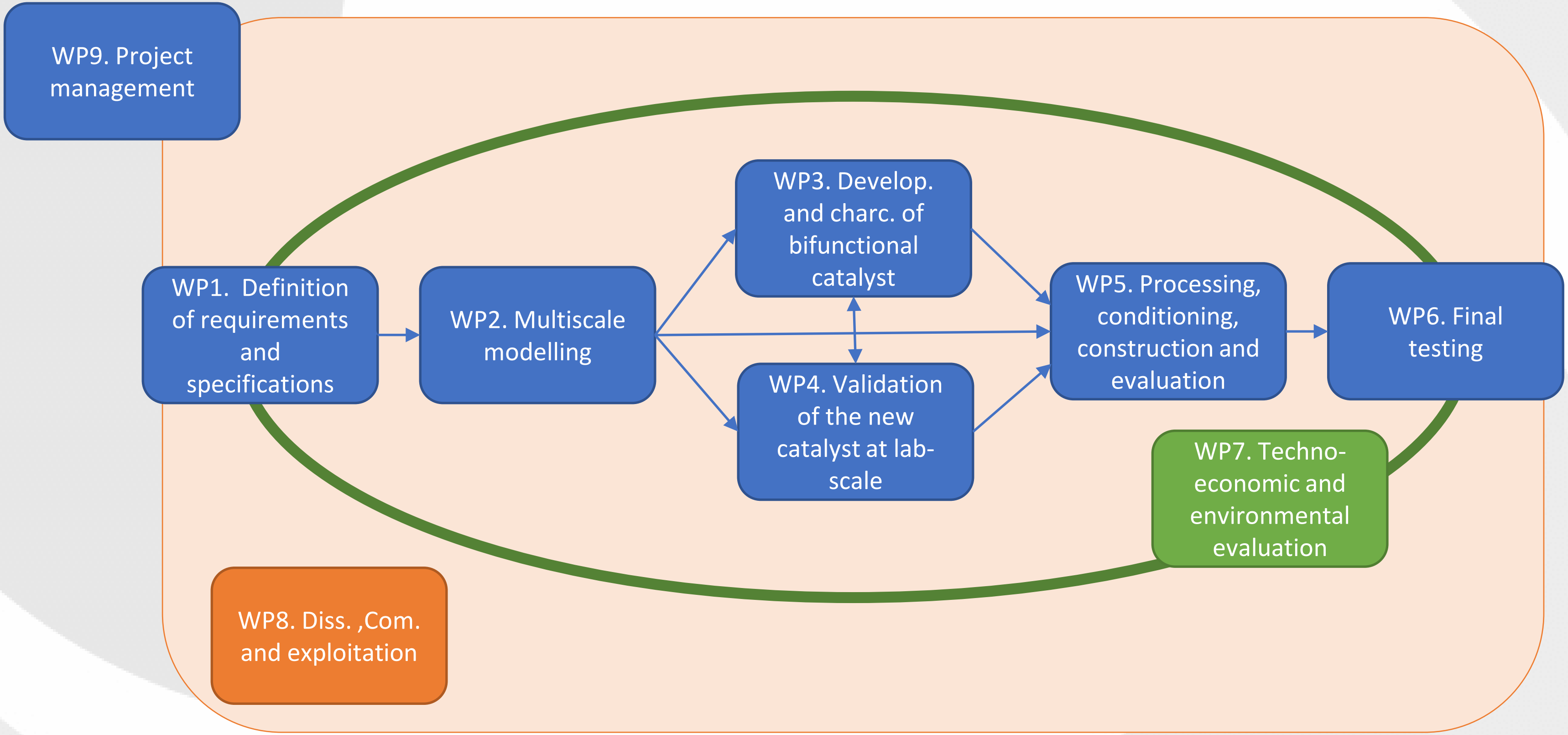
Implementation



Implementation



Implementation



5 Partners

Partners


3D-cat
TU/e
vito
Lurederra
centro tecnológico
TECNAN
TECNOLOGÍA NAVARRA DE NANOPRODUCTOS, S.L.
[TECHNOLOGY CENTRE] CARTIF
idener
SCIENTIFIC COMPUTING
Kneia
cnrs
DCS
COMPUTING
HELLENIC
PETROLEUM
aptL
BIOENERGY
NIGRITAS S.A.

6 Where are we?

Where are we?

ZEOCAT-3D

Year 1	Year 2	Year 3	Year 4

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42

WP1 **M1-M6**

WP2: Multi-scale modelling **M1-M34**

WP3: Development and characterization of bifunctional catalyst **M5-M33**

WP4: Validation of new catalyst at lab-scale **M13-M36**

WP5: Processing and conditioning **M5-M38**

WP6: Final testing **M27-M40**

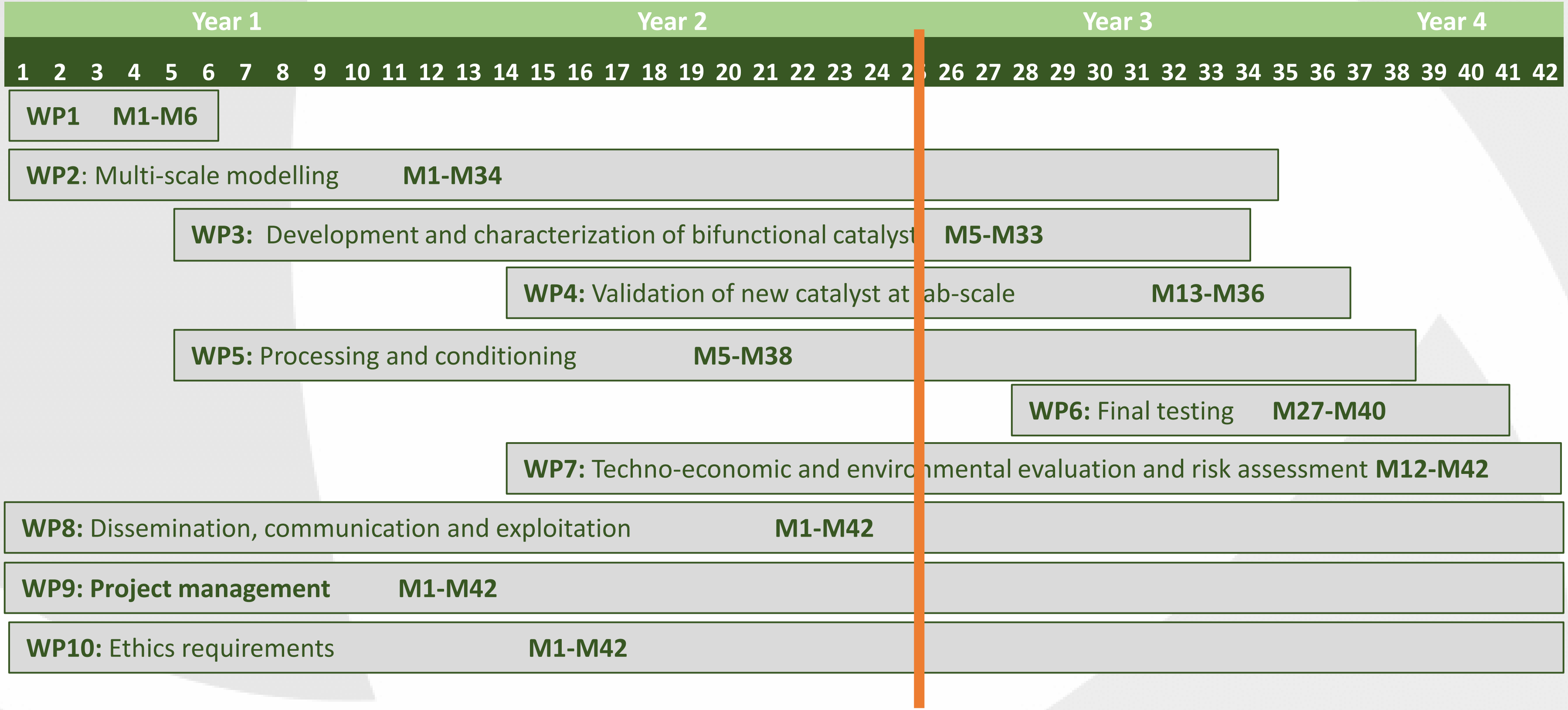
WP7: Techno-economic and environmental evaluation and risk assessment **M12-M42**

WP8: Dissemination, communication and exploitation **M1-M42**

WP9: Project management **M1-M42**

WP10: Ethics requirements **M1-M42**

Where are we?



Year 1
Year 2
Year 3
Year 4
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42
WP1 M1-M6
WP2: Multi-scale modelling M1-M34
WP3: Development and characterization of bifunctional catalyst M5-M33
WP4: Validation of new catalyst at lab-scale M13-M36
WP5: Processing and conditioning M5-M38
WP6: Final testing M27-M40
WP7: Techno-economic and environmental evaluation and risk assessment M12-M42
WP8: Dissemination, communication and exploitation M1-M42
WP9: Project management M1-M42
WP10: Ethics requirements M1-M42

Where are we?

Year 1 | Year 2 | Year 3 | Year 4

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42

WP1 **M1-M6**

WP2: Multi-scale modelling **M1-M34**

WP3: Development and characterization of bifunctional catalyst **M5-M33**

WP4: Validation of new catalyst at lab-scale **M13-M36**

WP5: Processing and conditioning **M5-M38**

WP6: Final testing **M27-M40**

WP7: Techno-economic and environmental evaluation and risk assessment **M12-M42**

WP8: Dissemination, communication and exploitation **M1-M42**

WP9: Project management **M1-M42**

WP10: Ethics requirements **M1-M42**

24 / 55 Deliverables submitted (18 accepted by the Commission)

First milestone planned for M28

Thank you

Any questions?

María Tripiana Serrano

maria.tripiana@idener.es