Multi-objective optimization of a sustainable ternary mortar for 3D printing

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Introduction

Cement production : **4-8%** of global greenhouse gas emissions [1]

Concrete 3D printing : material reduction

Fig 1. Example of 3D printing application (XtreeE).

Tab 1. Different 3DP concrete mixes cement content [2].

Concrete type	Study	OPC [kg/m³]
Standard concrete	Normal	~275
	Concrete masonry unit	~240
	High performance	~375
3DP concrete 1K	Le et al. 2012	532
	Kazemian et al. 2017	489
	Tay et al. 2019	639
	Nerella et al. 2020	525
	Chen et al. 2020	532
	Rushing et al. 2019	437
	Mechtcherine et al. 2019	438

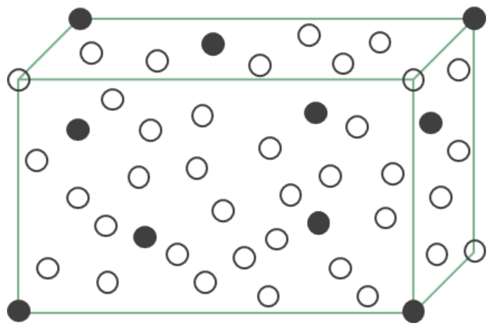
For 1K systems (unaccelerated concrete) :

- Rheological constraints
- Non-linear behavior with increasing number of parameters

Objective

Proposition of an automated reproducible methodology for reducing the environmental impact of 3D printing materials

- Application to a mortar with very low cement content



Materials

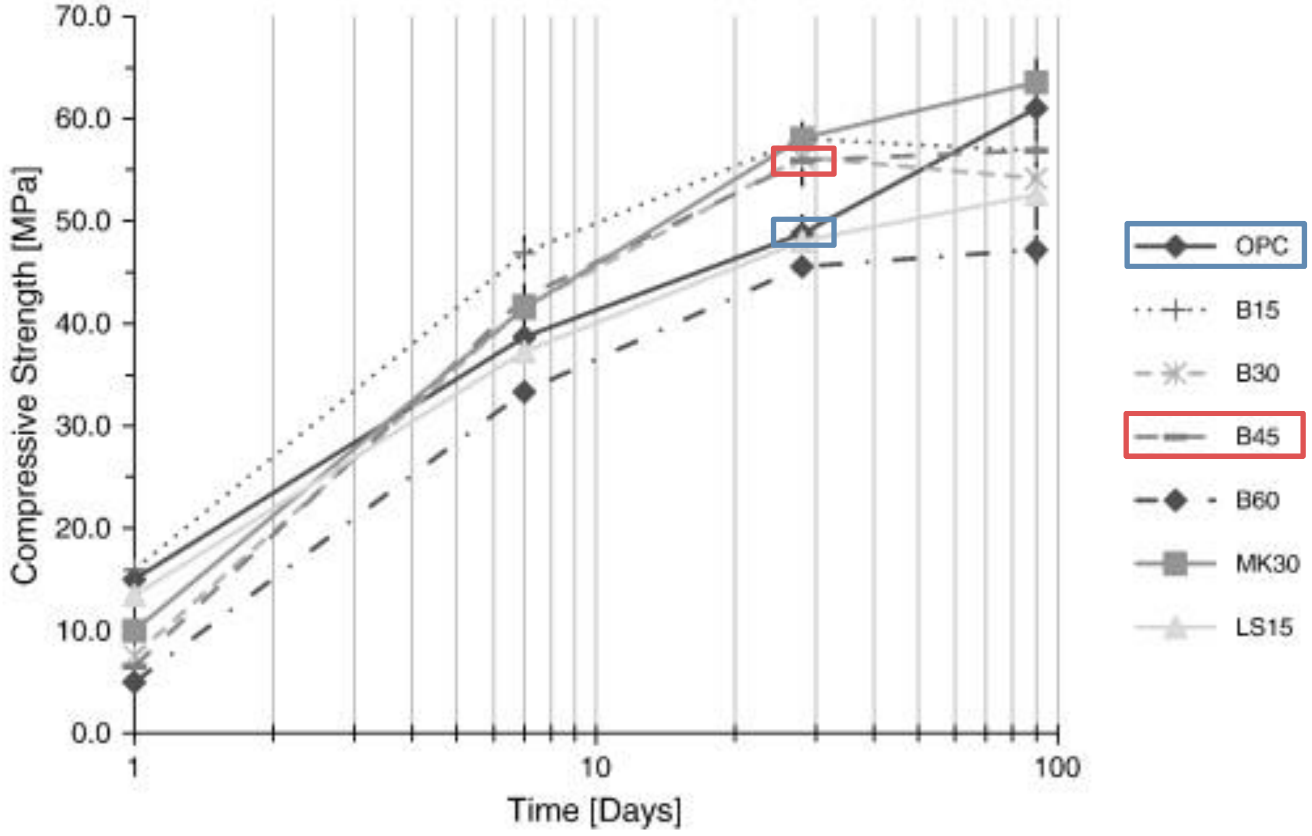


Fig 2. Compressive strength of blends mortars at 1, 7, 28 and 90 days [3].

Limestone calcined clay cement (**LC3**) :

- Greater cement substitution potential

→ *<u>B45</u> : 55% OPC / 30% calcined clay / 15% limestone filler*

- Relevance of process for higher number of parameters

Tab 2. Materials used in this study with abbreviations

Material	Abbreviation	Supplier	Comments
Cement	GUbSF	Ciment Québec (223km)	GU with 8% silica fume
Calcined clay	CC	Whitemud Resources (2900km)	80% metakaolin
Limestone filler	LF	Graymont (209km)	
Water	W		
Sand	Sa	Bomix (17km)	
Superplasticizer	SP	Master Builders (10km)	PCE

Methods

Large-scale 3D printing

Literature

Physical

Printability

Strength

LCA

Brightway2

Activity-browser

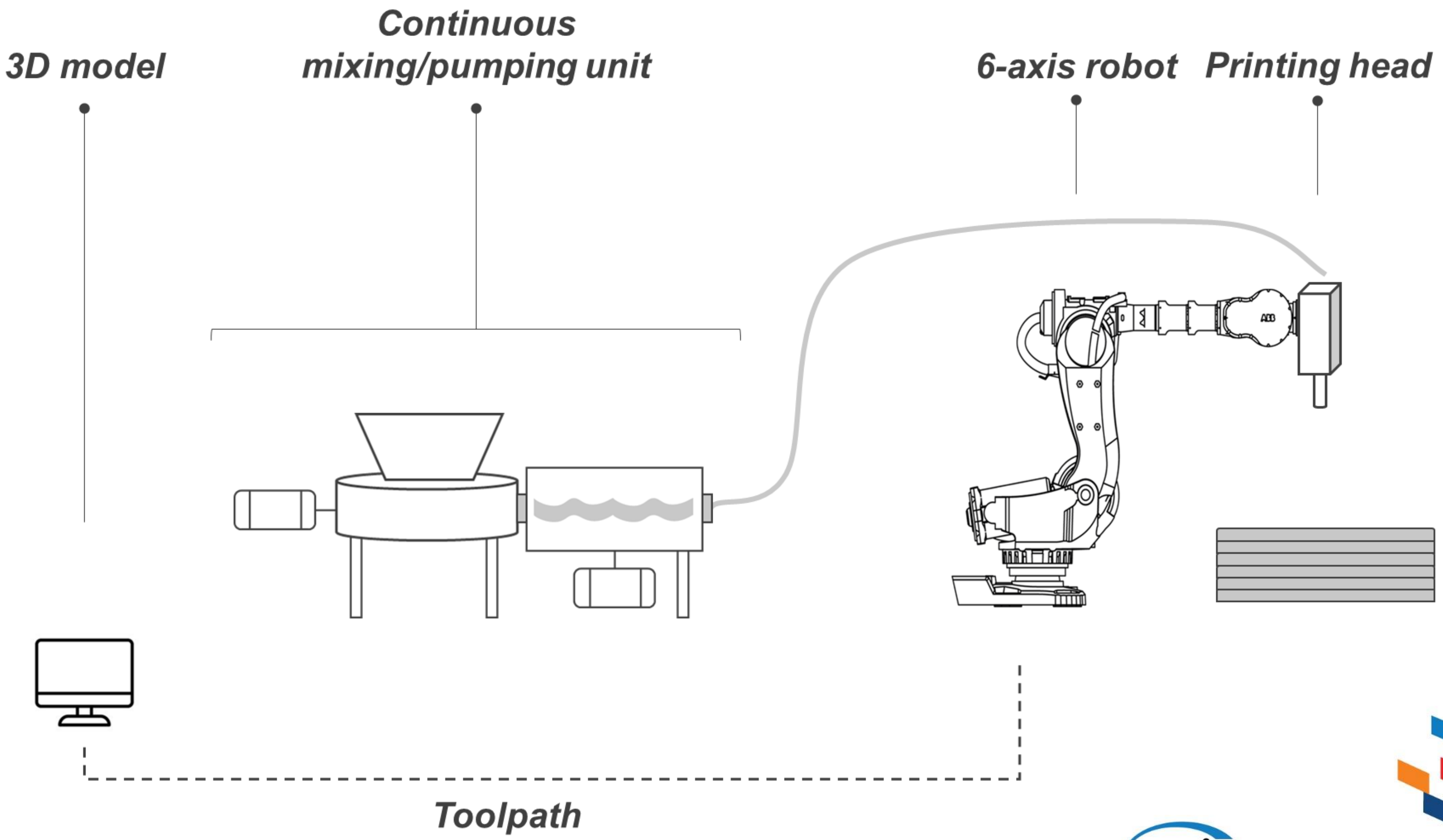
Ecoinvent 3.7 Cutoff

Optimization

Neural networks

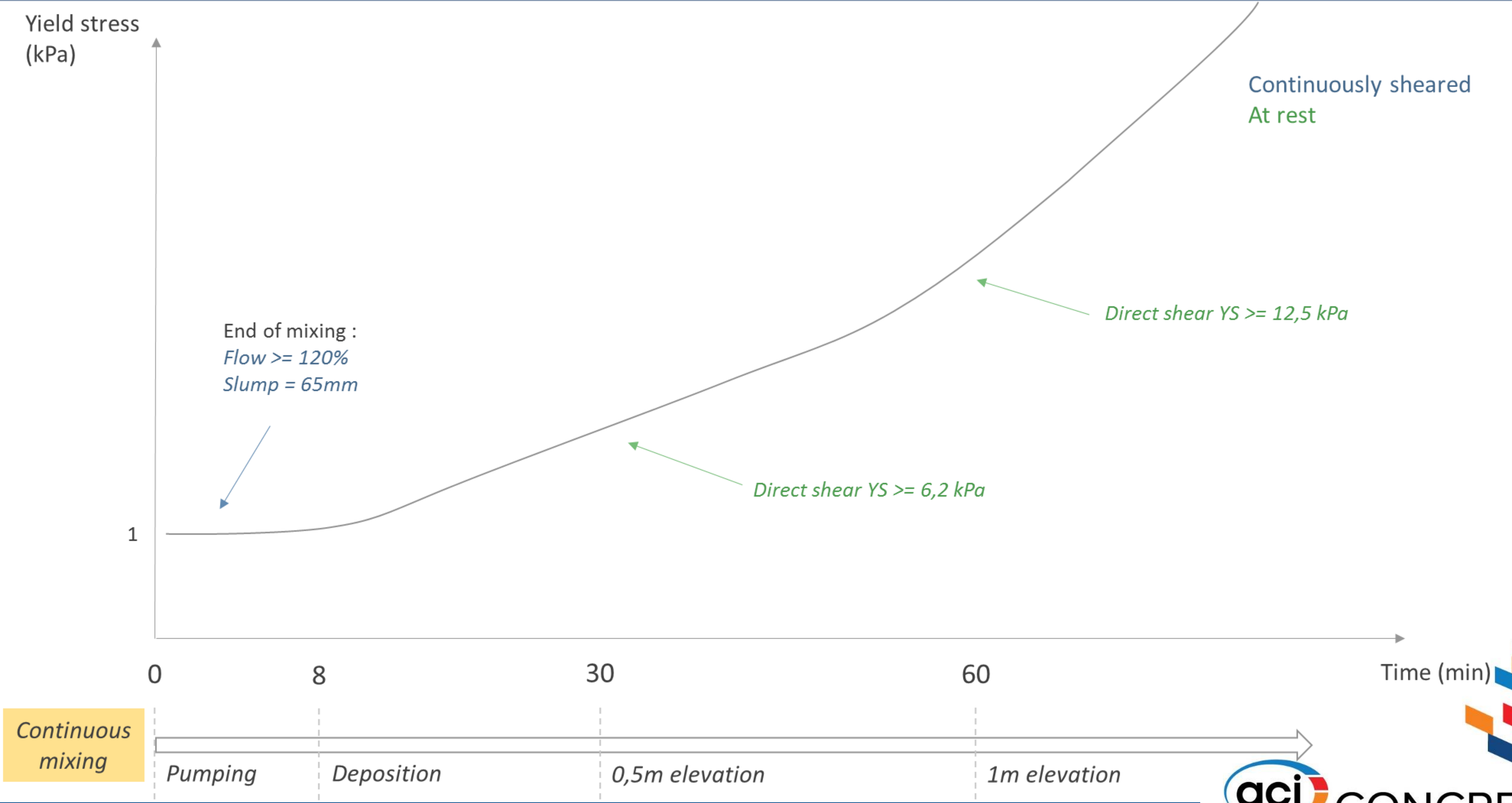
Non-dominated sorting algorithm

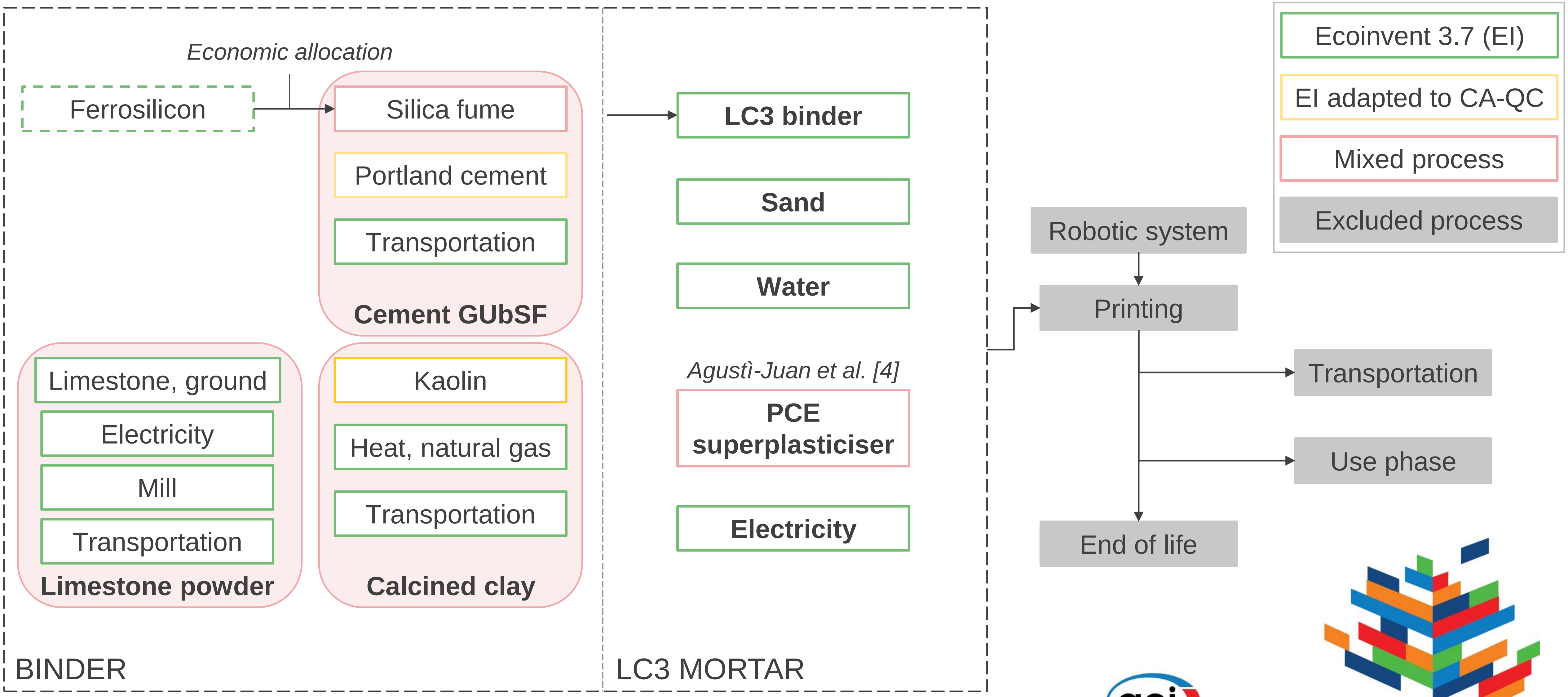
Python


3D model
Continuous mixing/pumping unit
6-axis robot
Printing head
Toolpath

Printability

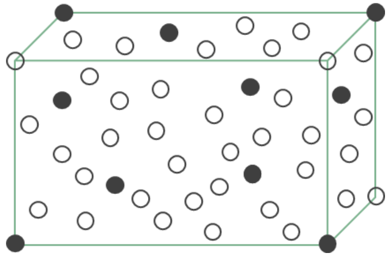
Flowability	Flow test
Shape retention	Slump test
Buildability	Direct shear test


Yield stress (kPa)
Continuously sheared
At rest
Direct shear YS >= 12,5 kPa
End of mixing :
Flow >= 120%
Slump = 65mm
Direct shear YS >= 6,2 kPa
1
0
8
30
60
Time (min)
Continuous mixing
Pumping
Deposition
0,5m elevation
1m elevation


Economic allocation
Ferrosilicon
Silica fume
Portland cement
Transportation
Cement GUbSF
LC3 binder
Sand
Water
Agustì-Juan et al. [4]
PCE superplasticiser
Electricity
Limestone, ground
Electricity
Mill
Transportation
Limestone powder
Kaolin
Heat, natural gas
Transportation
Calcined clay
BINDER
LC3 MORTAR
Robotic system
Printing
Transportation
Use phase
End of life
Ecoinvent 3.7 (EI)
EI adapted to CA-QC
Mixed process
Excluded process

Optimization process

Based on Sergis and Ouellet-Plamondon, Digital Discovery, 2022



	Flow	Slump	Athix
Mix 1	x %	x mm	x Pa/s
Mix …	…	…	…

NN Flow | NN Slump | NN Athix

Trained

Parameterized LCA model

Evaluation

NSGA-II

Ranking of non-dominated solutions

Selection – crossover – mutation

Uniformely distributed set of Pareto optimal solutions

Selection of 3 solutions for validation

Iterations

Results : Reference material




Objective : lower the climate change score while maintaining printability constraints

120 %

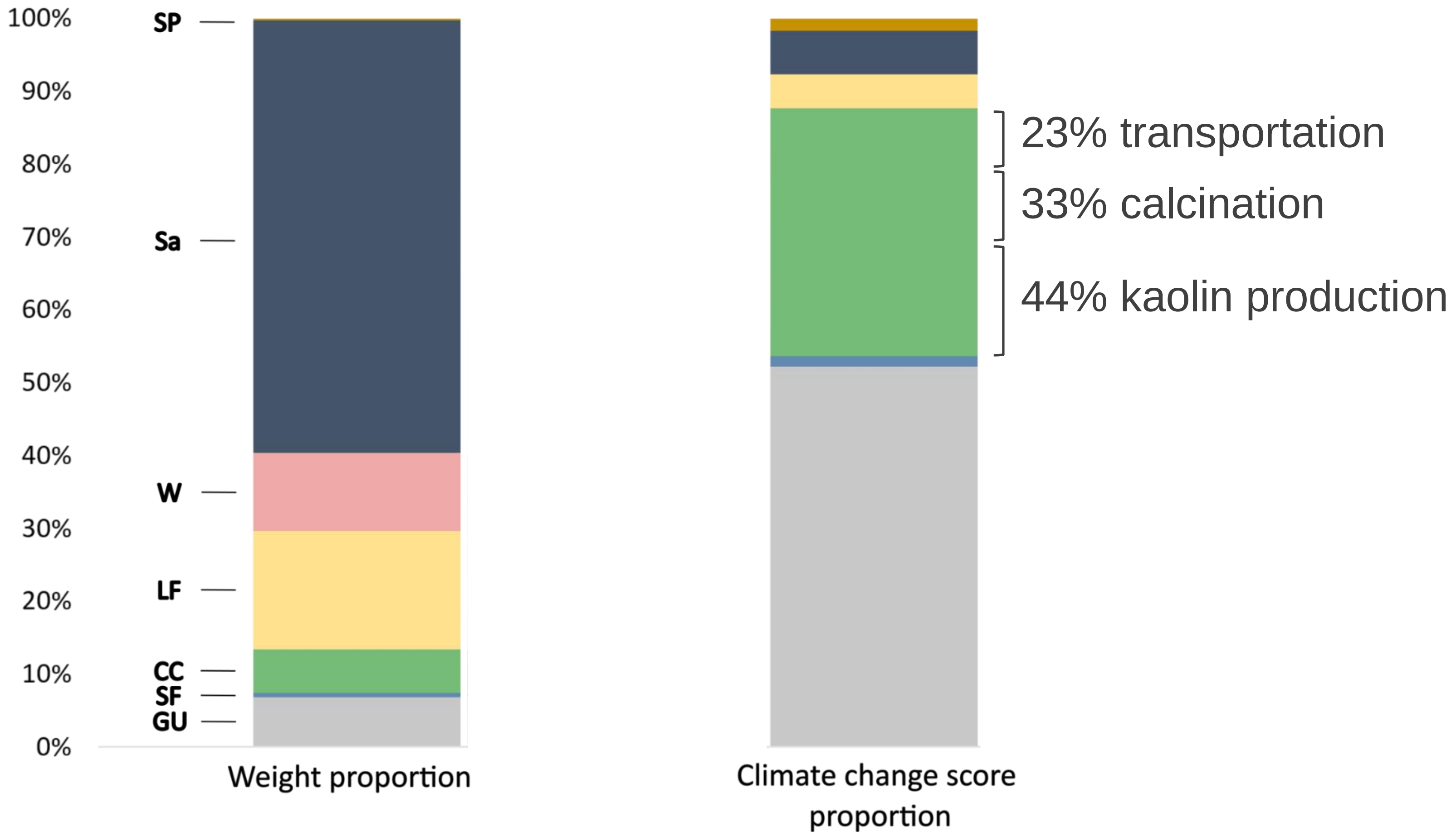
67 mm
2.6 in

3.6 Pa/s

30.5 MPa

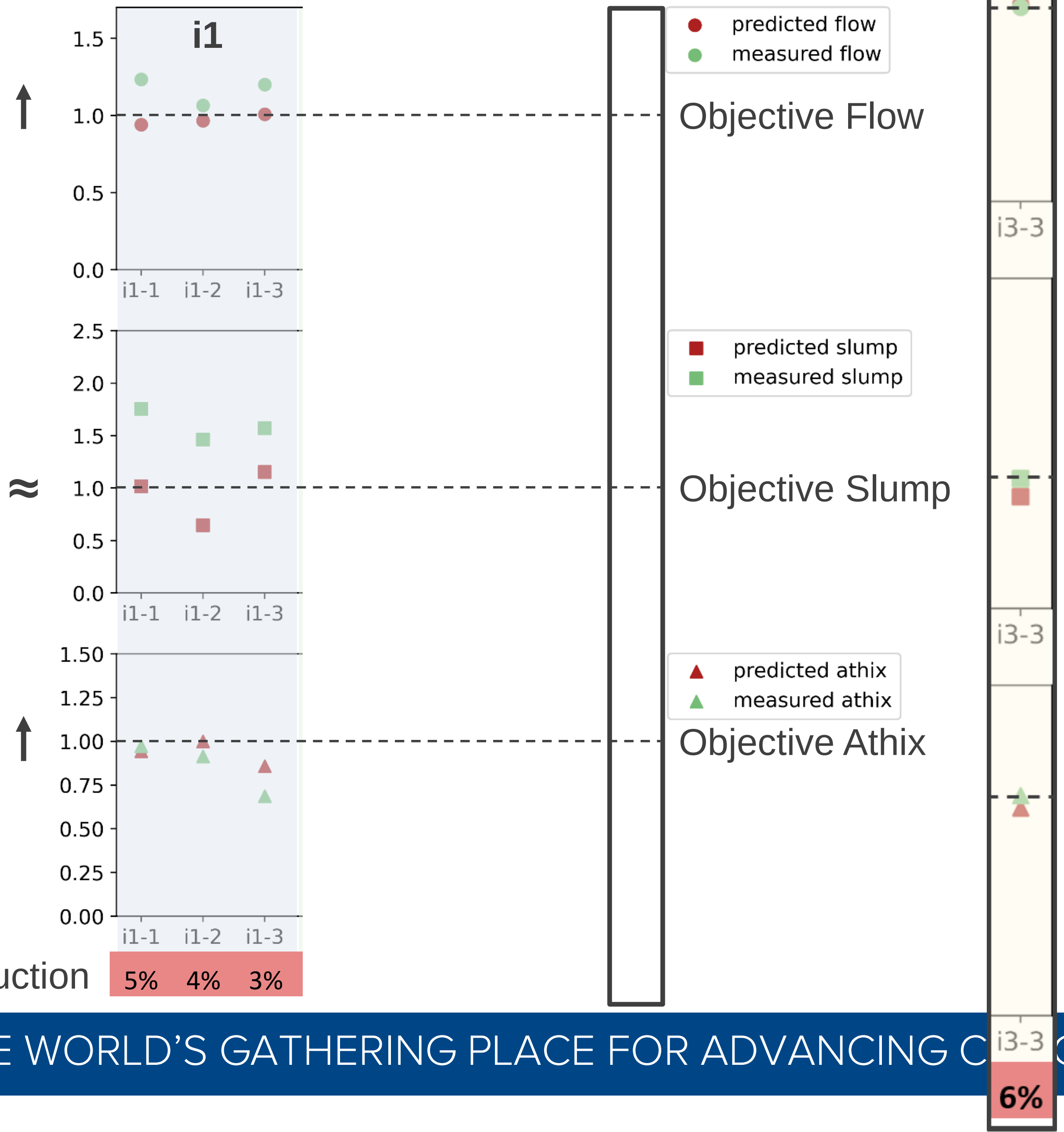
251 kgCO_2-eq/m^3

Results : Global warming potential



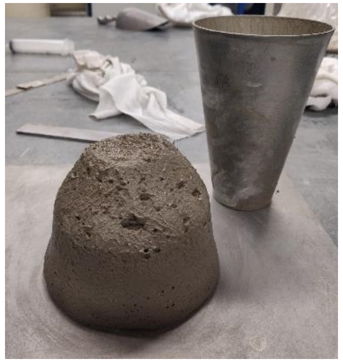
Main contributors to climate change score :

- **Cement 53%**
- **Calcined clay 34%**



GWP reduction 5% 4% 3%

120 %

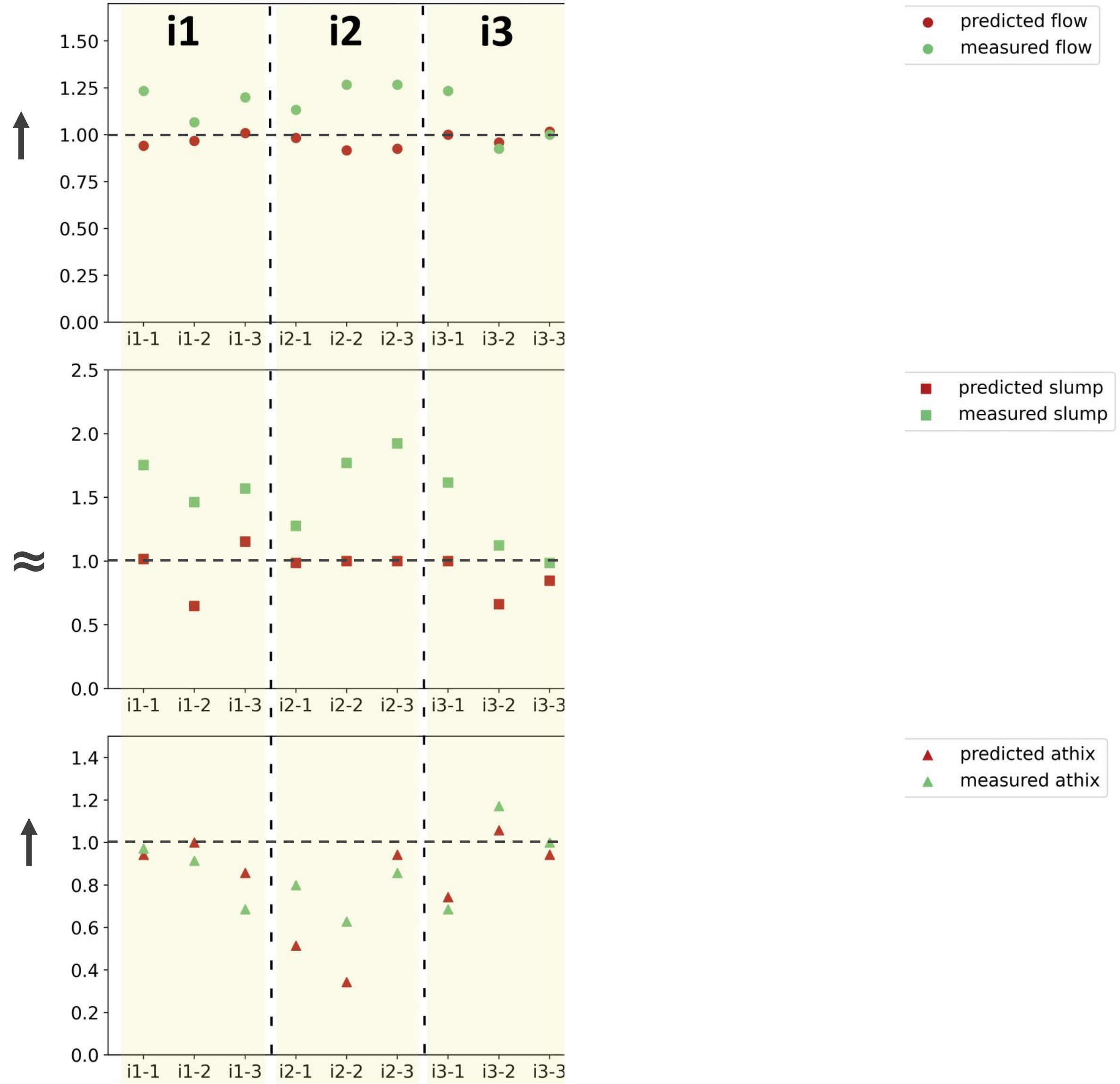


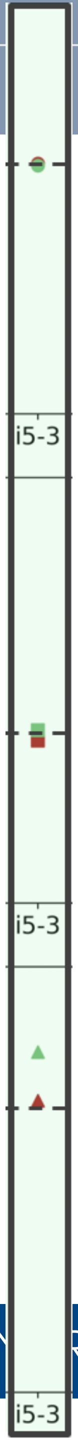
64 mm
2.52 in

Athix : 3.5 Pa/s

236 $kgCO_2$-eq/m^3

Effective process for reducing the GWP of complex materials





119 %

66 mm
2.60 in

Athix : 4.2 Pa/s

226 kgCO_2-eq/m^3

Discussions

- **Minimization of cement content**
- **Optimization of calcined clay content**

- In the LCA model : **Conservative modeling of calcined clay**
  - Calcination in rotary kiln with natural gas
  - Electricity mix of CA-SK for the production of kaolin →
  - Transportation distance of 2900 km

658 kgCO_2-eq/ton
High estimation !

Discussions

- Reference material → already effective
- Restricted bounds for mixture parameters
- **6-parameter** optimization with **4-6 objective functions :**
  - **Dataset size** → Expected substantial error in the first iterations

Conclusion

- The methodology reduces the number of mixes necessary for material optimization, especially for GWP reduction :
  – Efficient way to take the environmental impact into consideration in the mix design

- Reproducible with **locally sourced materials / customizable objectives**

- Possibility to include the compressive strength in order to **switch objectives** :
  – Next step : Identify 40 MPa 3D printing mortar with minimized climate change score

References

1. Andrew, R. M. “Global CO_2 emissions from cement production,” Earth System Science Data, V. 10, No. 1, 2018, pp. 195–217.

2. Flatt, R. J., and Wangler, T. “On sustainability and digital fabrication with concrete,” Cement and Concrete Research, V. 158, 2022, p. 106837.

3. Antoni, M., Rossen, J., Martirena, F., Scrivener, K. “Cement substitution by a combination of metakaolin and limestone,” *Cement and Concrete Research*, V. 42, No. 12, 2012, pp. 1579–89.

4. Agustí-Juan, I., and Habert, G. “Environmental design guidelines for digital fabrication,” Journal of Cleaner Production, V. 142, 2017, pp. 2780–91.

5. Sergis, V., and Ouellet-Plamondon, C. M. “Automating mix design for 3D concrete printing using optimization methods,” Digital Discovery, 2022, p. 10.1039.D2DD00040G.

Thank you !

Questions ?

Annex

(wt%)	GUbSF	CC	LF
SiO_2	27.0	62.5	2.21
Al_2O_3	4.2	31	0.37
Fe_2O_3	1.6	1.1	0.14
CaO	57.5	0.4	53.6
MgO	1.6	0.3	0.51
SO_3	3.6	0	0.1
TiO_2	0	0.6	0.01
Na_2O	0	0.16	0.02
K_2O	0	1.81	0.13

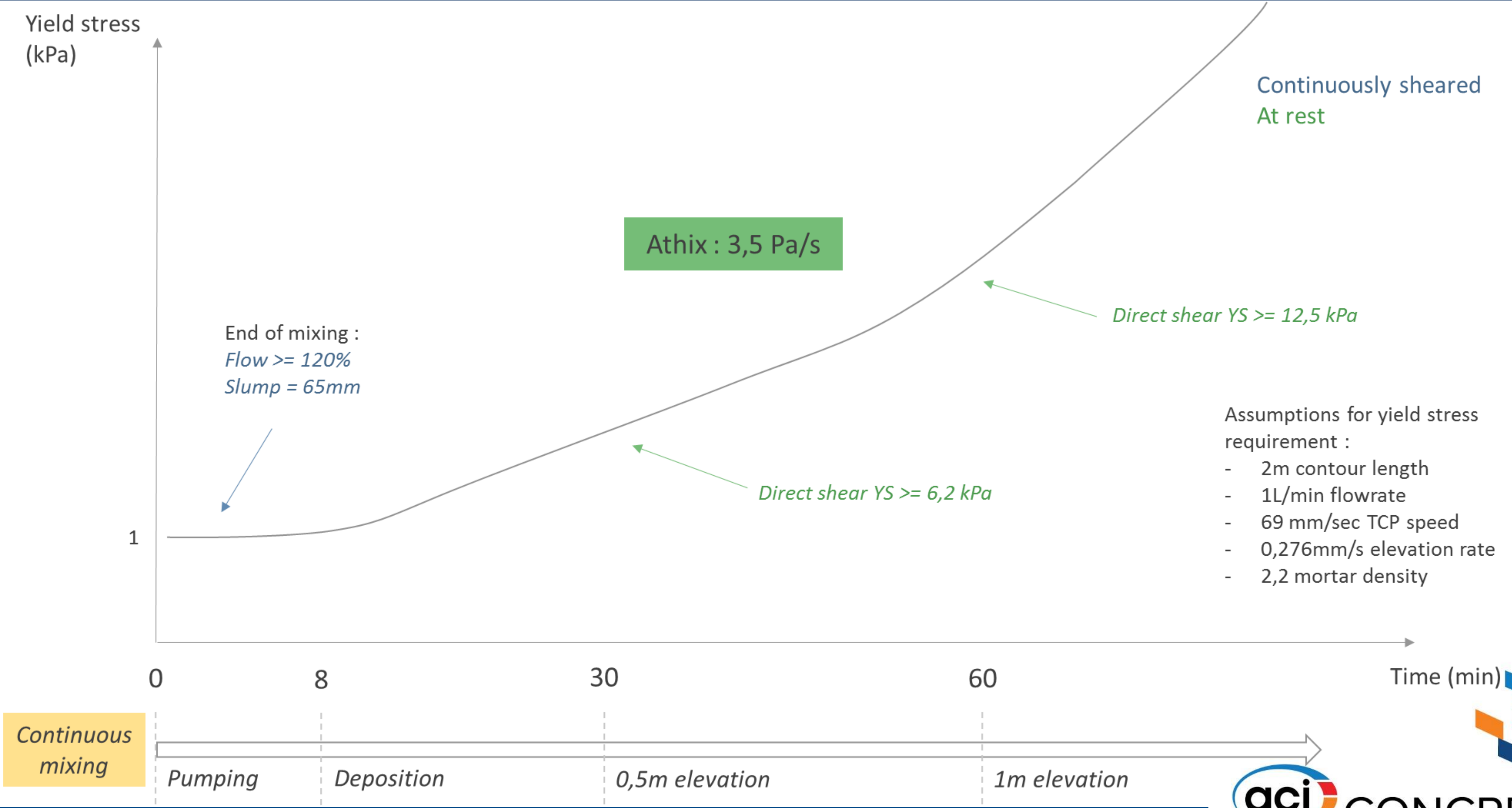
Fig. Chemical composition of binder components.

Sieve analysis

Sieve (mm)	% passing
2.5	100
1.25	85 - 95
0.630	70 - 86
0.315	50 - 65
0.160	15 - 25
0.080	0 - 3

Tab. Sieve analysis of Bomix sand.

Annex



Assumptions for yield stress requirement :

- 2m contour length
- 1L/min flowrate
- 69 mm/sec TCP speed
- 0,276mm/s elevation rate
- 2,2 mortar density

$$\tau = \frac{\rho g H}{\sqrt{3}}$$

Annex

104%

65mm

Annex

```
R^2 and RMSE for ALL data:  [0.9454113, 13.019289]

R^2 and RMSE for TEST data:  [0.9666956, 10.664082]

TEST data predictions:
             x    y
0    98.274605   82
1   128.040039  110
2   113.283371   88
3   142.720413  131
4   127.655396  132
5   123.745049  126
6   123.376373  116
7   125.034515  120
8   102.442924   90
9   120.483849  118
10   90.725113  111
11   -0.391596    0
12   -0.343865    0
13   -0.279409    0
14    6.924143    0
15   -0.450232    0
16  143.865829  152
17  153.782120  152
18   -0.431078    0

ANN model summary:

Best solution found:
[{'act_f': 0, 'n_hidden': 4, 'lay_1': 147, 'lay_2': 356, 'lay_3': 62, 'lay_4': 210, 'lay_5': 392, 'lay_6': 17, 'learn_r': 0.0021192779443649145}, array([11.031])]

Model: "sequential_4581"
```

Results of ANN training singe objective optimization for flow (i5)

Annex

NSGA-II

Random population P_0 — *N sets of parameters*

↓ P_0 *selection – crossover – mutation*

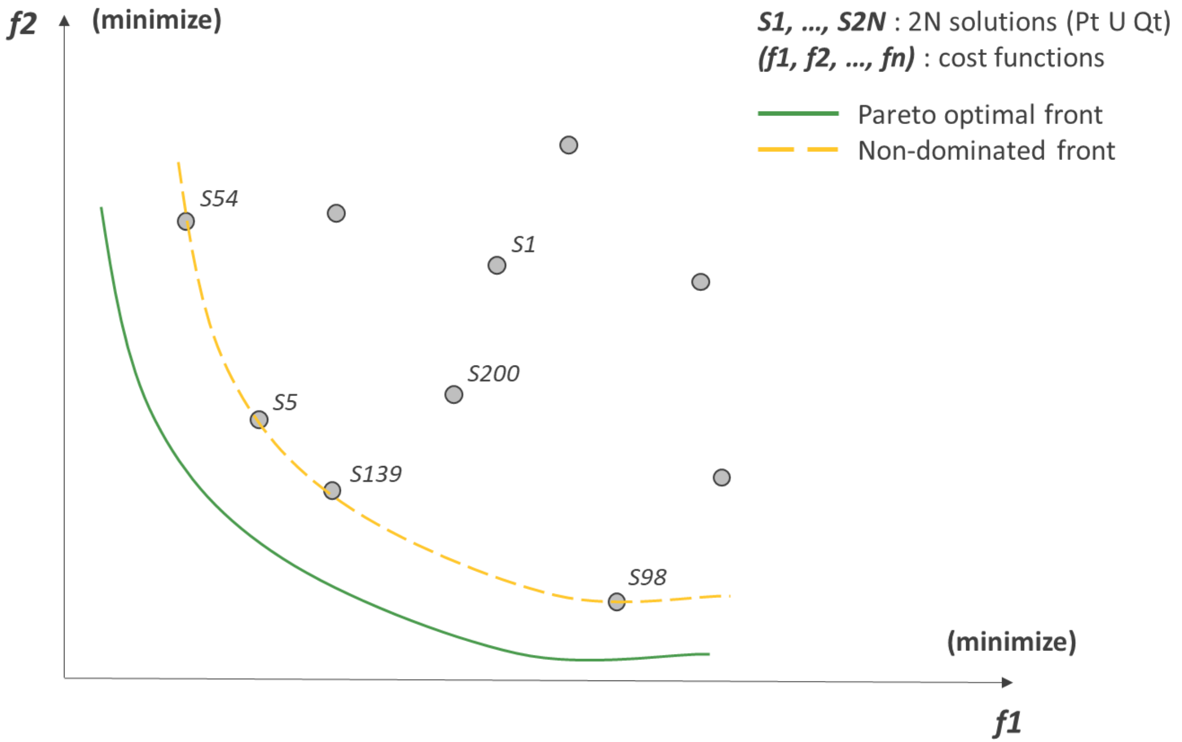
Iteration t — Child population Q_t

↓ Ranking of non-dominated solutions →
|
P_t *selection – crossover – mutation*

Iteration t+1 — Child population Q_{t+1}

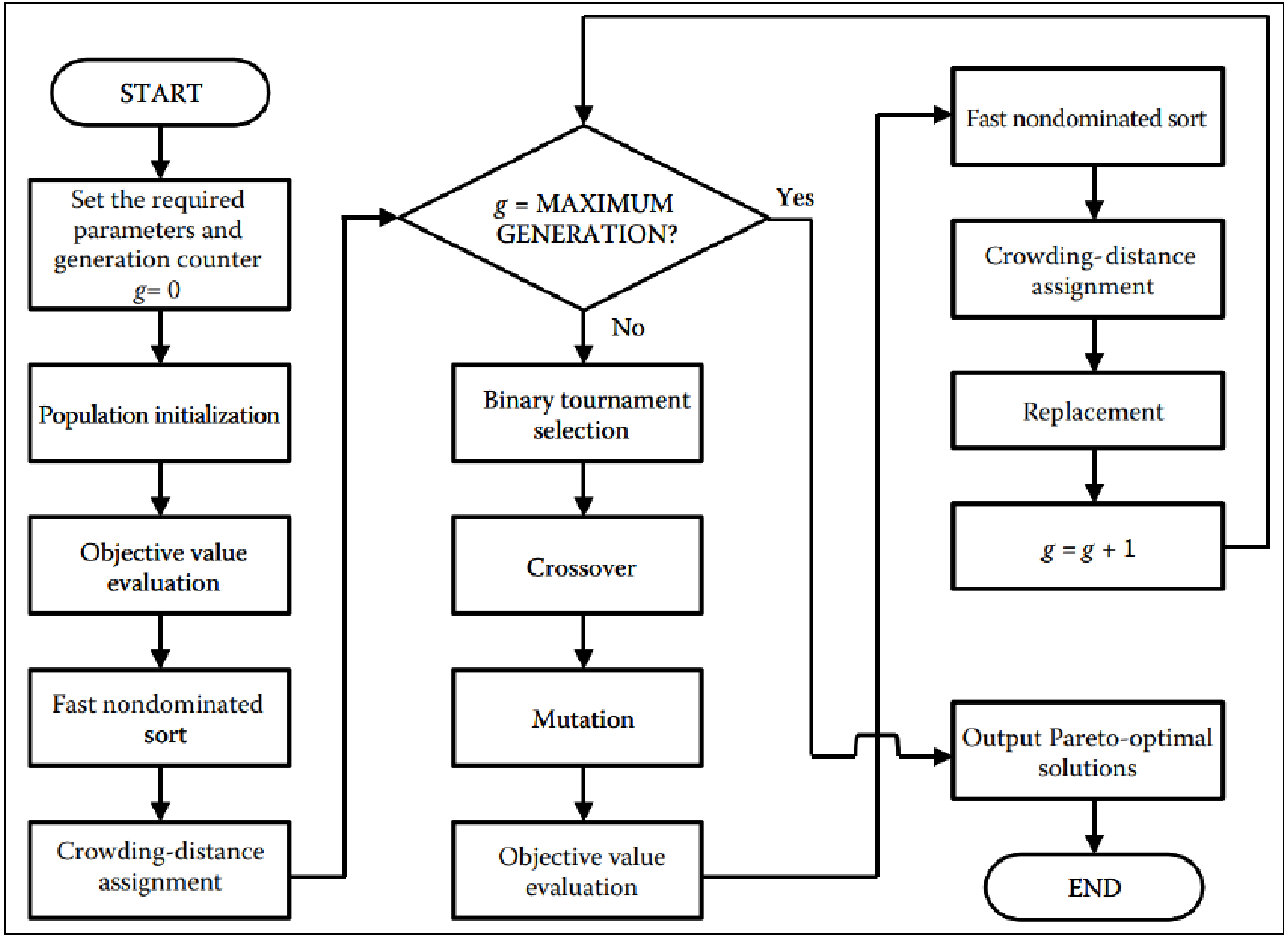
...

Uniformely distributed set of Pareto optimal solutions



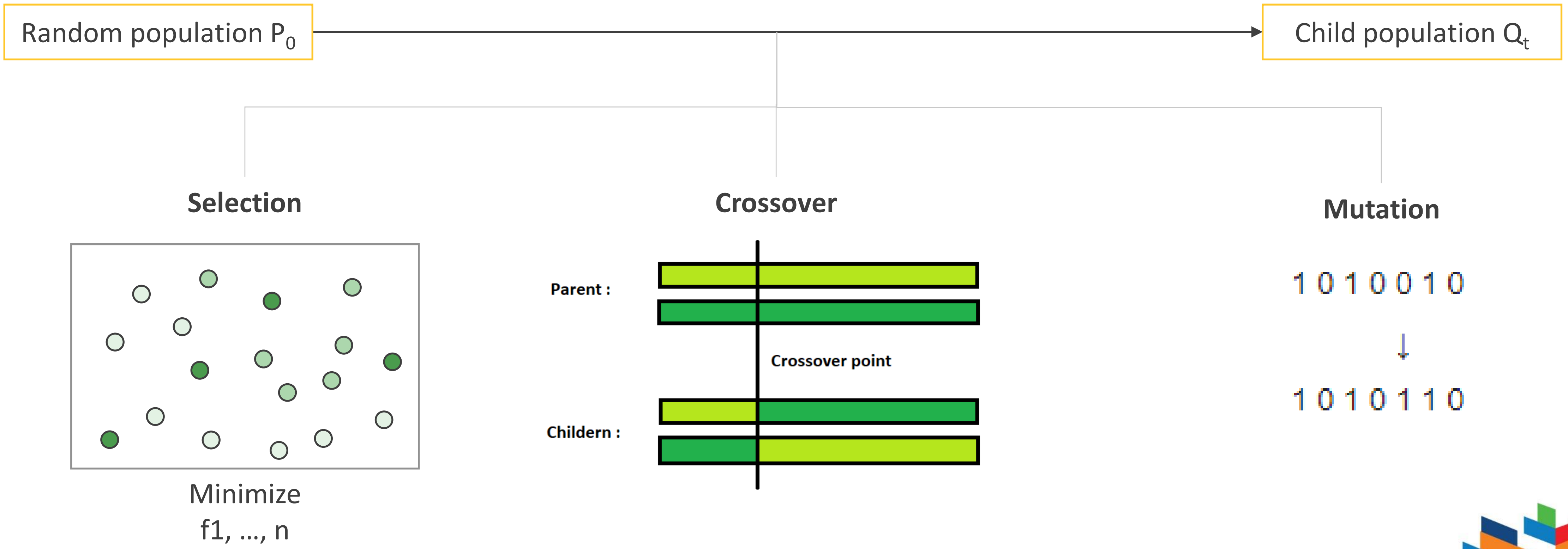
Objective space

Annex

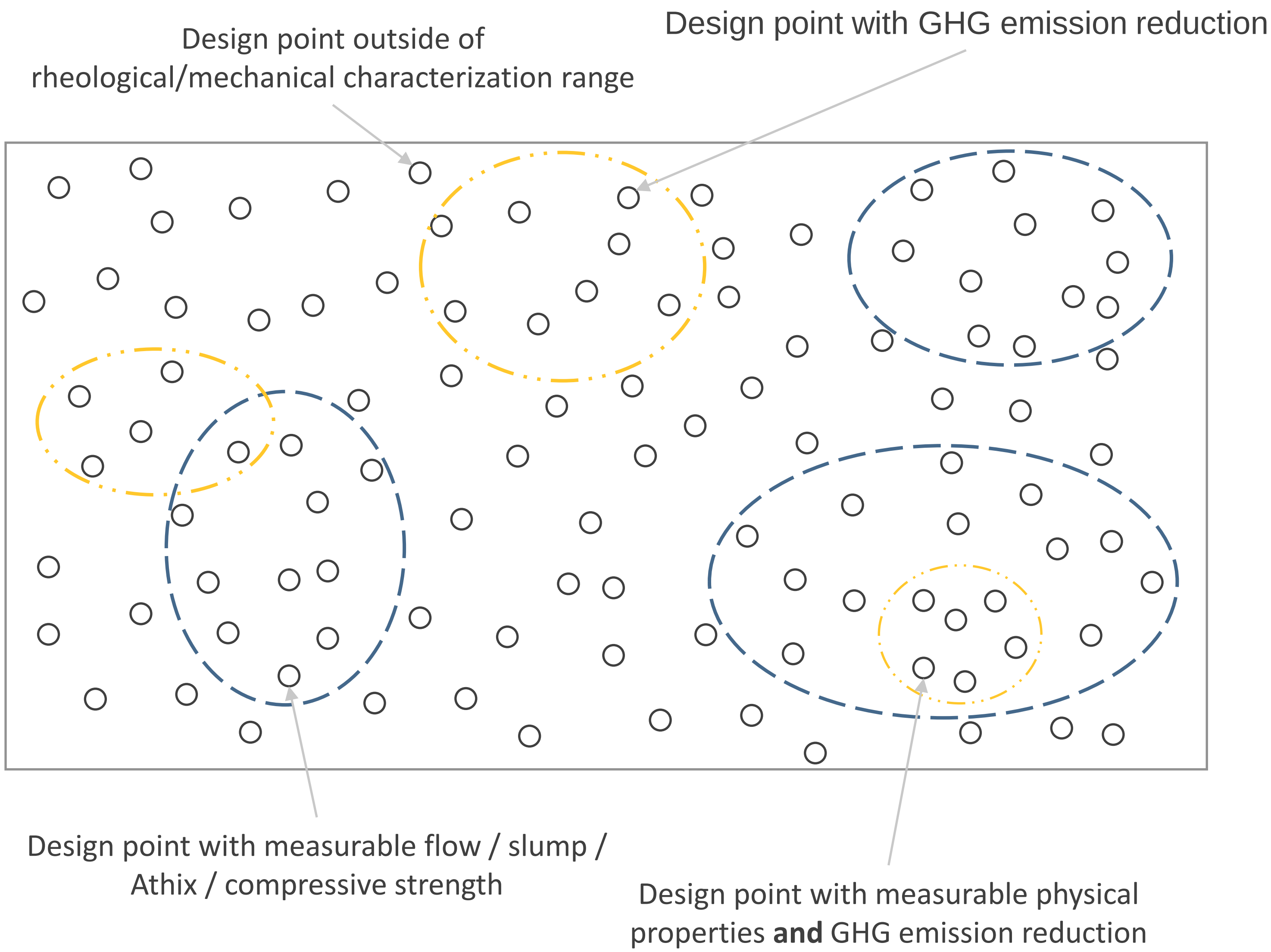


Tang et al. 2018 : A Fast Method of Constructing the Non-Dominated Set: Arena's Principle

Annex

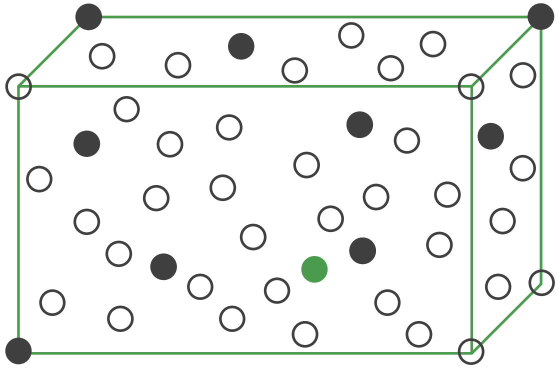

Random population P_0
Child population Q_t
Selection
Minimize
f1, …, n
Crossover
Parent :
Crossover point
Childern :
Mutation
1 0 1 0 0 1 0
1 0 1 0 1 1 0

Annex

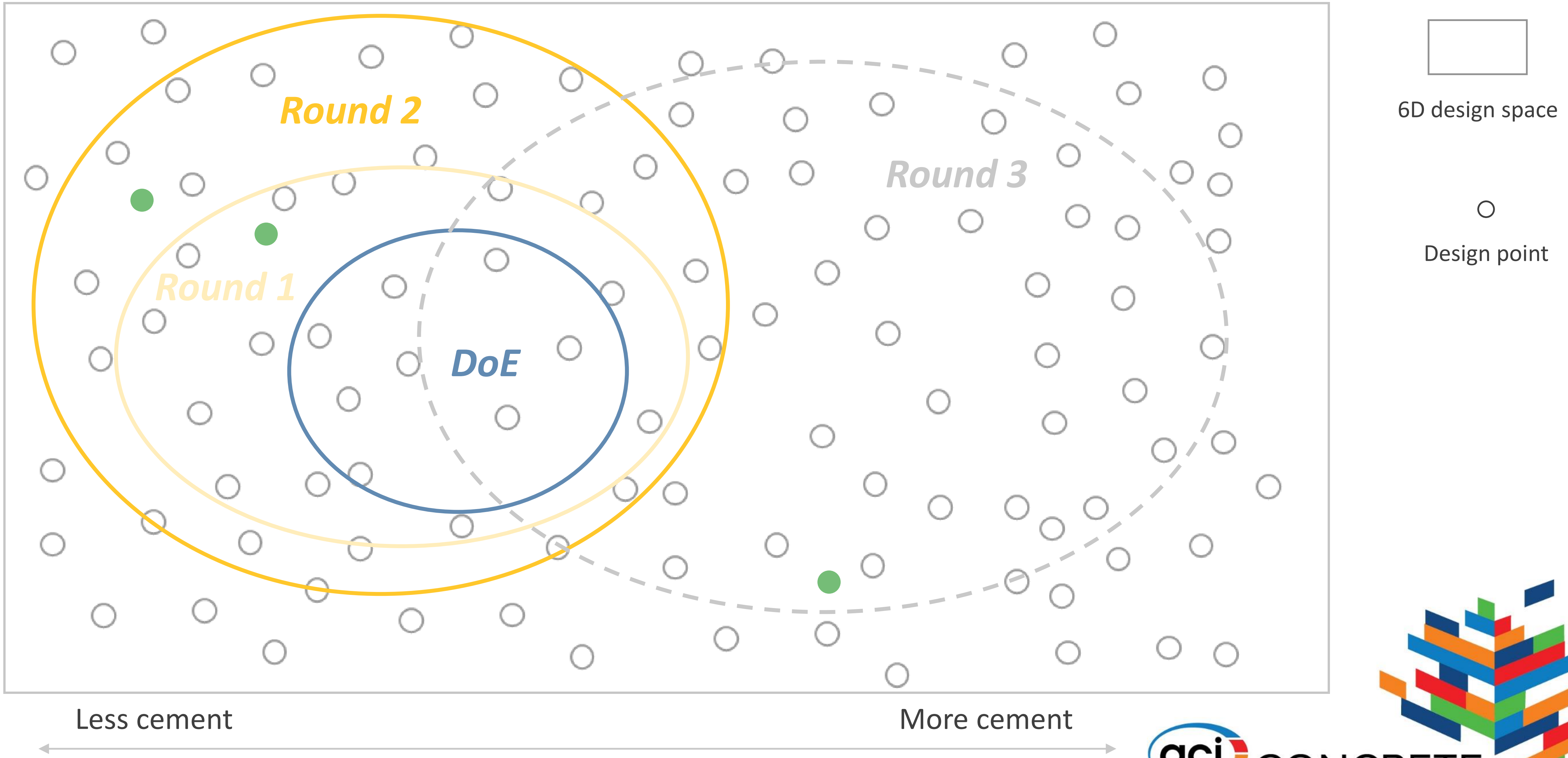


6D design space

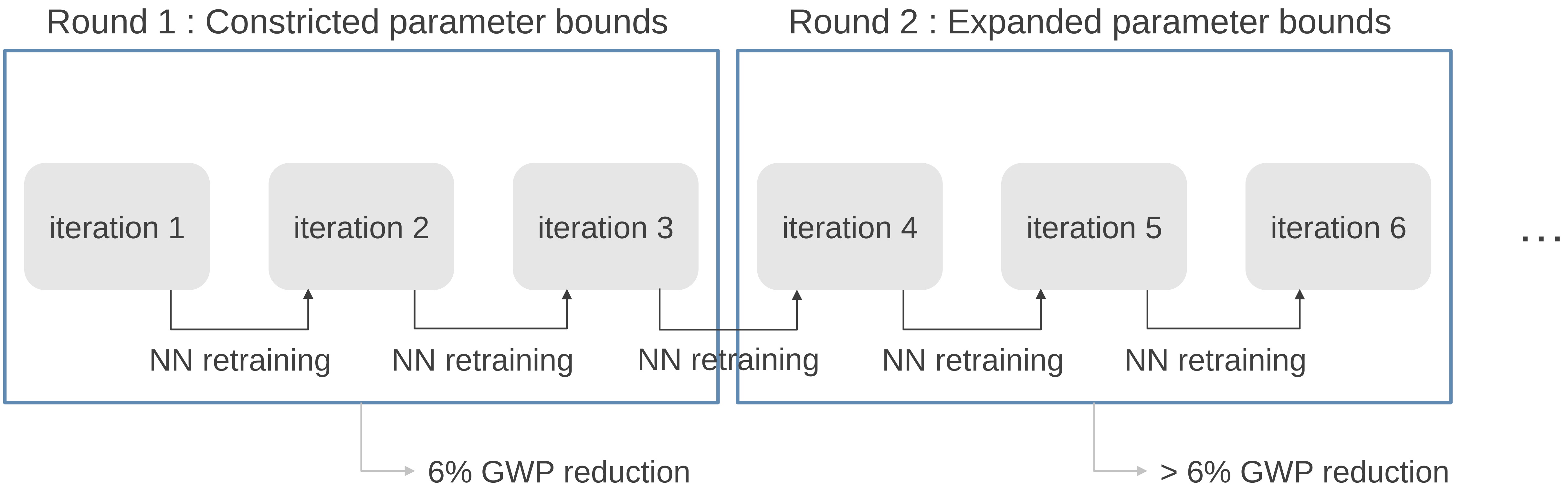
Design point : set of 6 values



Annex


Round 2
Round 3
Round 1
DoE
6D design space
Design point
Less cement
More cement

Annex



As the experiments progress, the predictions get more reliable
- This methodology is suited for local materials