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Design of core-shell aerogel particles combining AI tools and supercritical drying for oral drug delivery

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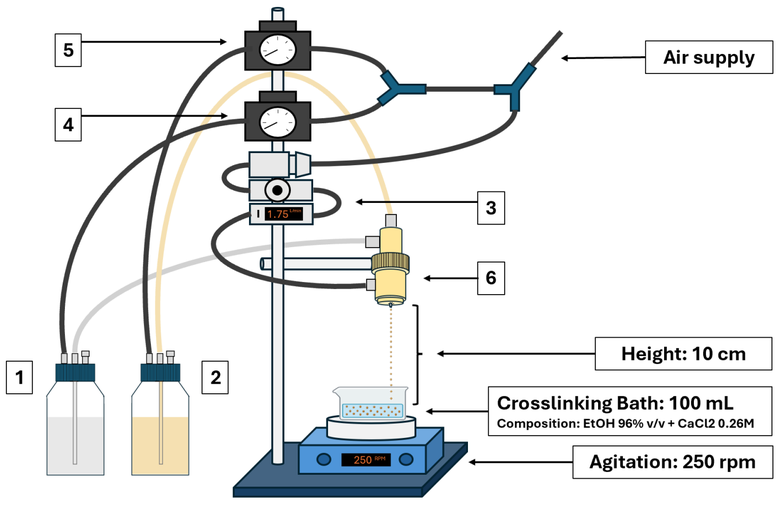
INTRODUCTION & AIM

Bioaerogels have been postulated as drug delivery systems, and can be synthesized via sol–gel processes using a wide variety of polysaccharides [1]. Core-shell aerogels can be prepared by combination of air-assisted coaxial dripping systems with subsequent supercritical drying [2]. This methodology involves numerous processing parameters, making Artificial Intelligence (AI) tools invaluable for optimizing and understanding the effect of each variable on the particle characteristics [2]. In this work, AI tools were employed to develop aerogel particles using alginate (Alg) solutions as drug-loaded cores and konjac glucomannan (KGM) solutions as coatings.

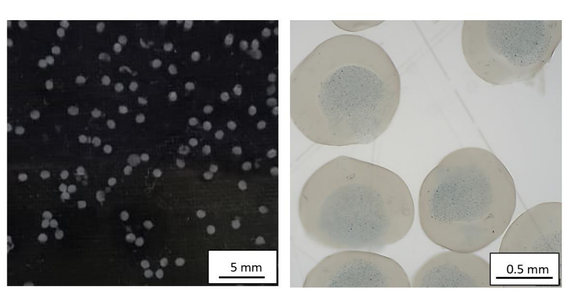
METHOD

Processing parameters selected to model the formulation method:

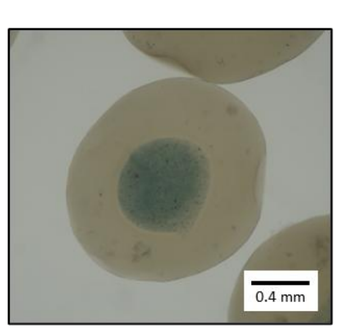


1. [KGM] = 0.6 – 0.7% w/v
2. [Alg] = 0.75 – 1.25% w/v
3. Airflow = 1.75 – 2.65 L/min
4. Pressure (KGM) = 0.4 – 1.2 bar
5. Pressure (Alg) = 0.2 – 1.0 bar
6. Nozzle configuration = 0.8/0.35, 0.5/0.15, 0.8/0.15 mm

Selected example of an evaluated formulation to obtain explicative models and optimal formulations:

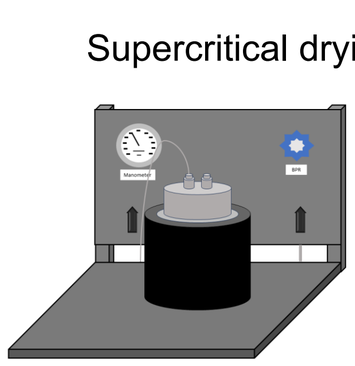


1. Feret diameter (mm)
2. Circularity (Values: 0-1)
3. Coating thickness (mm)
4. Core position (score)
5. Nozzle blockage (score)
6. Core volume (mm³)



Optimal formulation!

Supercritical drying conditions:



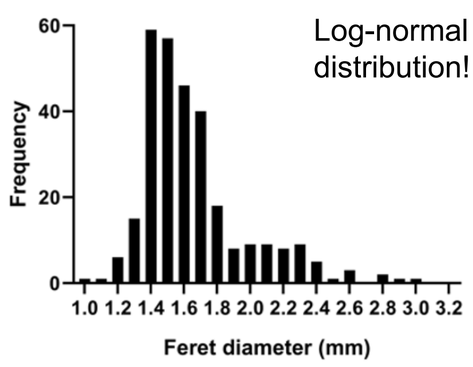
Pressure: 120 bar
Temperature: 40ºC
Time: 5 h (4 h dynamic + 1 h static)

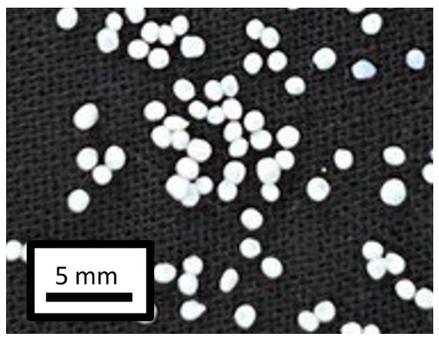
RESULTS & DISCUSSION

Morphological and textural properties of final aerogel formulations

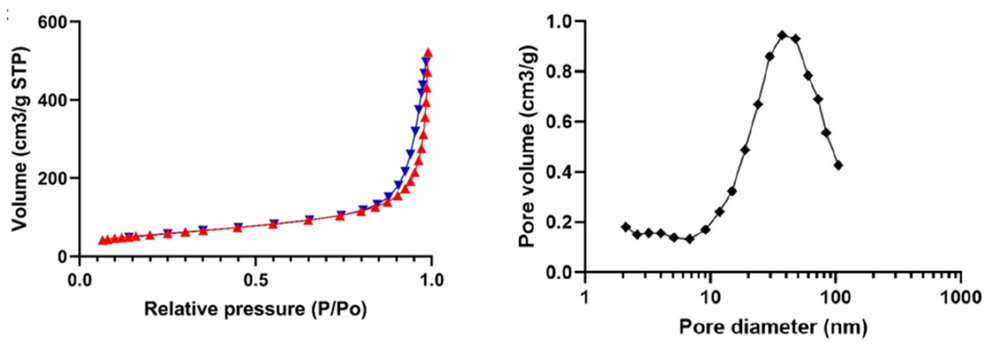
D_{Feret} (mm)	Geometric deviation	Circularity	A_{BET} (m^2/g)	V_p (cm^3/g)	D_p (nm)	ρ_{skel} (g/cm^3)
1.77	1.21	0.83	201 ± 10	0.78 ± 0.04	15.4 ± 0.8	1.71 ± 0.01

Size distribution and picture of the core–shell aerogel formulation

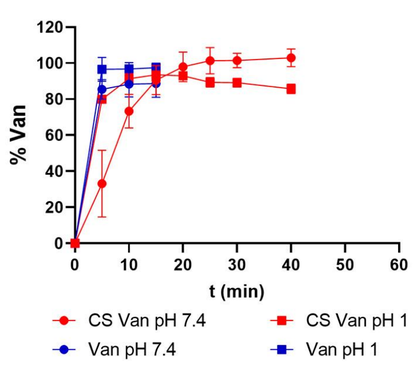


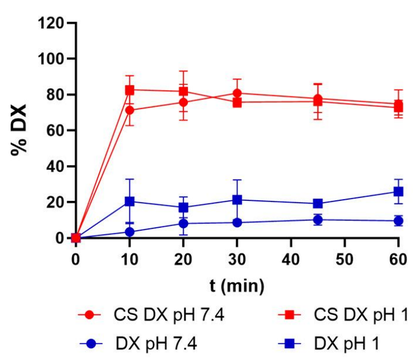


Isotherm and mesopore size distribution of core–shell aerogels



Drug loading (DL %), Entrapment Yield (EY %) and drug release of Vancomycin (Van) and Dexamethasone (DX) from core–shell aerogels





	DL (%)	EY (%)
Aerogels (van)	11.7 (2.8)	17.3 (3.3)
Aerogels (DX)	0.032 (0.001)	0.182 (0.003)

CONCLUSIONS

- It was possible to produce core–shell gel particles based on alginate and konjac glucomannan in a one-step process.
- AI enabled the optimization of the core–shell particle production process.
- Core–shell aerogels loaded with lipophilic drugs facilitated instantaneous drug release.
- The obtained formulations were unable to modulate the release of hydrophilic drugs.

ACKNOWLEDGMENTS

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[1] F. De Cicco, P. Russo, E. Reverchon, C.A. García-González, R.P. Aquino and P. Del Gaudio. Carbohydrate Polymers, 147, 482-489 (2016).

[2] C. Illanes-Bordomas, M. Landin and C.A. García-González, Polymers, 17, 1919 (2025).