

D3.1. Simulation model of the microwave pyrolysis

FLEXBY

FLEXIBLE AND ADVANCED BIOFUEL TECHNOLOGY THROUGH AN INNOVATIVE MICROWAVE PYROLYSIS & HYDROGEN-FREE HYDRODEOXYGENATION PROCESS

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Author(s):	Saeed Kooshki	
Contributor(s):	Mumtaz Ali Ansari, Loges Christoph, Ogrzall Jerome	
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EXECUTIVE SUMMARY

This deliverable outlines the simulation-driven design of a custom microwave-assisted pyrolysis reactor, a core component of the FLEXBY project focused on converting biogenic waste into renewable biofuels. Using CST Studio Suite and material data from T2.1, detailed electromagnetic simulations were conducted to define the applicator's geometry, dimensions, and microwave coupling configuration.

Key design specifications were established, covering material properties (e.g., specific heat capacity, dielectric loss factors), throughput, temperature-time profiles, atmospheric conditions, operating mode (batch or continuous), loading/unloading methods, and control system requirements. The specifications for the flexible general-purpose system were defined with contributions from technical partners CSIC, US, IDENER, and PMI.

The reactor features a two-stage configuration—microwave drying followed by pyrolysis under a nitrogen atmosphere—and integrates innovations such as a spiral antenna for field uniformity, advanced control algorithms, and safety systems including hydrogen leak detection. Simulation results validated efficient thermal behavior and process control, forming a robust foundation for prototyping and integration into the FLEXBY workflow.



1. INTRODUCTION

The FLEXBY project aims to advance a novel thermochemical process for converting biogenic residues—namely, microalgae cultivated in domestic wastewater and industrial oily sludge from the dairy industry and the Agar-Agar industry (macroalgae processing industry)—into renewable biofuels. Although initial project plans considered oily sludge from refinery operations as a potential feedstock, this was later excluded. As documented in Deliverable D2.1 (CSIC), GALP, a project partner, indicated that it could not provide suitable samples due to the bio-based nature required for the final products. Consequently, CSIC sourced four alternative industrial sludge samples from other sources in Asturias, Spain. The six final residues used in the project—two from dairy industry sludges, two from macroalgae processing, and two microalgae-derived—were fully characterized for suitability.

Central to this initiative is the development of a custom-designed microwave-assisted pyrolysis reactor by FRIMA, intended to transform these feedstocks into three primary outputs: bio-liquid, pyro-gas, and bio-char. The reactor employs a controlled electromagnetic environment to achieve efficient thermal decomposition of the input material.

This report presents the simulation-driven development of a batch-mode microwave pyrolysis reactor, with the objective of maximizing material conversion efficiency while ensuring process stability and scalability in line with FLEXBY's production targets. Key aspects of the reactor design include characterization of electromagnetic field behavior, assessment of temperature-dependent dielectric properties of feedstocks, and optimization of microwave energy distribution to achieve uniform and controlled heating.

The design process began with the formulation of a preliminary reactor model, based on collaborative input from all technical project partners (CSIC, US, PMI, IDENER, A4F) and informed by key feedstock parameters: moisture content, bulk density, and processing scale. This initial design served as the foundation for simulation-based optimization.

A detailed electromagnetic simulation framework was developed using CST MICROWAVE STUDIO Suite¹, incorporating empirical dielectric data to model both electromagnetic field distribution and heating response within the reactor chamber.



Simulation outcomes guided iterative adjustments to the reactor geometry, applicator configuration, and material interfaces to enhance heating uniformity and energy efficiency.

Alongside the physical design optimization, the process architecture was defined. Specification of sensor systems, control logic, and safety mechanisms were included. Given the production of flammable pyro-gases, safety considerations—such as thermal containment, pressure regulation, and gas monitoring—were integrated into both the hardware and control system design from the outset.

This report details the simulation methodology, model parameters, and key findings that inform the reactor's final design and its alignment with the overarching objectives of the FLEXBY project.



2. METHODOLOGY FOR SIMULATION, DESIGN, AND PROCESS EXECUTION

The methodology followed in this study involved a structured sequence of experimental characterization, conceptual design, simulation, and optimization to develop a microwave-assisted pyrolysis system for macroalgae biomass. This approach enabled accurate modeling of the heating behavior and informed the development of a safe, efficient microwave reactor system tailored for the FLEXBY project. An integral part of the methodology was the coordination of multiple technical meetings with key project partners—CSIC, US, PMI, and IDENER—to collaboratively define system requirements and design specifications. These meetings clarified critical aspects such as feedstock parameters, safety constraints, instrumentation needs, and integration with control systems, ensuring that the final reactor design aligned with both project objectives and partner expectations.

2.1. Dielectric Characterization of Macroalgae Feedstock

To understand the interaction between microwave energy and biomass, the dielectric properties of all samples were measured using a high-temperature dielectric characterization system. The goal was to quantify the relative permittivity (ϵ') of the feedstock at 2.45 GHz, the standard frequency used in microwave processing. More detailed information on the measurement procedures and results is provided in Deliverable D2.1, and is not repeated here to avoid redundancy.

2.2. Conceptual Design and Process Flow

Based on dielectric results and the process requirements, a conceptual reactor design and process scheme were developed. The system was configured for batch processing, optimized for maximum 2 kg of sample per cycle.

The process was divided into two main stages:

• Stage 1: Microwave Drying – Moisture removal from the biogenic waste under operator control, using microwave energy based on moisture content and dielectric behavior.



• Stage 2: Microwave Pyrolysis – The dried feedstock is further heated under microwave radiation to reach up to 700 °C, initiating pyrolysis reactions.

An inert nitrogen (N_2) atmosphere was continuously maintained during both stages to prevent oxygen infiltration and ensure safety, stability, and controlled pyrolytic conversion.

2.3. Electromagnetic Simulation and Reactor Optimization

Using CST Studio Suite, a comprehensive simulation of the reactor cavity was performed to optimize the electromagnetic field distribution for uniform heating and high energy efficiency.

Simulation objectives included:

- Maximizing field uniformity within the biomass bed.
- Minimizing hotspots and thermal gradients.
- Ensuring minimal reflected power and effective coupling.
- Integrating thermal and electromagnetic performance for real-world batch conditions.

Waveguide placement, cavity dimensions, and material interfaces were iteratively refined. Safety features such as waveguide chokes, absorbing loads, and sealing mechanisms were also modeled to eliminate microwave leakage and comply with industrial standards.

Initially, a high-temperature dielectric characterization of all samples was performed to estimate their relative permittivity (ϵ ') and loss tangent (tan δ) following an approach commonly applied in microwave engineering. These measurements, summarized in D2.1 (table 7), were carried out to obtain approximate dielectric properties necessary for electromagnetic (EM) simulations and subsequent microwave system optimization.

Typically, such experimentally obtained values are directly utilised in full-wave electromagnetic (EM) simulations to guide the design and optimization of microwave-assisted processes. However, the samples available for dielectric characterization exhibited moisture contents ranging from 5% to 15%, which is considerably lower than



the target operational range for microwave drying and pyrolysis, where moisture levels can reach up to 85%. To address this limitation, dielectric property data corresponding to higher moisture levels were sourced from peer-reviewed literature and verified online databases^{2,3}. These values, representative of sludge with elevated moisture content, are compiled in Table 1 and were used to simulate more realistic process conditions.

Additionally, it is important to note that the sample volume within a container changes as a function of its moisture content, directly influencing the effective sample height during microwave exposure. This variation, detailed in Table 1, was incorporated into the simulation models to ensure accurate boundary conditions and improved predictive performance.

It should also be clarified that parameters such as heat capacity and enthalpy of vaporization were not analysed in this study, as they are not required for electromagnetic field distribution simulations. The primary objective was to optimize the microwave energy absorption and heating uniformity, which can be effectively achieved using accurate dielectric properties alone. Therefore, these thermal parameters were deemed unnecessary for the scope of this design-focused modelling.

Sludge Moisture %	Dielectric Constant	Loss Tangent	Sludge Height (mm)
80	45-55	0.45-0.55	75
60	35-45	0.35-0.45	60
40	25-35	0.25-0.35	50
20	10-20	0.15-0.25	40

Table 1. Feedstock Microwave Properties and Height Variation with Moisture Percentage^{2,3}.



3. **RESULTS**

3.1. Conceptual Design

The preliminary design concept of the microwave-assisted pyrolysis reactor, developed for the thermochemical processing of microalgae, is illustrated in Figure 1. The pre-design serves as the foundational framework for subsequent simulation studies aimed at optimizing the reactor's geometry and operational efficiency. The initial design parameters, as presented in the illustration, particularly the dimensions of the central glass reactor, were established to ensure suitability for practical handling, ease of cleaning, and process integration.



Figure 1. Preliminary design concept of a microwave-assisted pyrolysis reactor, operating in two stages: an initial drying mode followed by nitrogen (N_2) injection and pyrolysis processing.



The system is designed to carry out two primary process stages within a single, multifunctional reactor using microwave energy:

1. **Microwave Drying Phase:** In this stage, wet microalgae are introduced into the reactor and exposed to microwave heating to reduce their moisture content to levels suitable for subsequent processing steps (which will depend on the specific tests to be performed). Microwave drying enables uniform energy distribution and rapid moisture removal, offering a more efficient alternative to conventional thermal drying techniques. It is important to note that the optimal final moisture content of the sample will ultimately depend on the overall process conditions—both upstream and downstream. The FLEXBY process will evaluate different initial moisture levels to determine the most suitable wet content, once the full process parameters are finalized. Notably, the hydrodeoxygenation (HDO) step led by US may require a significant water content in the input material, which will influence the drying targets set during this stage.

2. Microwave Pyrolysis Phase: After sufficient moisture reduction, the system continues into the pyrolysis phase without the need for intermediate transfer. Under an inert N_2 atmosphere, the dried biomass undergoes thermal decomposition through sustained microwave heating. This process results in the production of value-added products such as bio-oil, syngas, and biochar.

The reactor pre-design described in this section was employed as the baseline configuration for simulation modeling. These simulations were conducted to evaluate the thermal and flow behavior within the reactor, with the goal of optimizing its dimensions for improved performance and scalability. Key design considerations included thermal distribution, residence time, microwave penetration depth, and ease of maintenance.

3.2. Electromagnetic Simulation

3.2.1. Antenna:

A circularly polarized spiral antenna backed by a pyramidal metallic enclosure is proposed for efficient microwave delivery, as illustrated in Figure 2(a)–(c). The antenna exhibits a return loss of approximately -12 dB at the operating frequency of 2.45 GHz in free space, indicating effective impedance matching. The circular polarization,



characterized by an axial ratio below 3 across the desired frequency band [Figure 2(d)], offers significant advantages over linearly polarized systems, such as improved field homogeneity and enhanced penetration depth, what results —beneficial for microwave processing of lossy and heterogeneous materials.

In contrast to conventional waveguide-based microwave launchers, the proposed antenna ensures more uniform energy distribution within the target medium. With a directivity of approximately 18 dBi [Figure 2(e)], the antenna effectively focuses microwave energy toward the sample, thereby enhancing power density at the point of interaction. Additionally, the antenna demonstrates broadband performance suitable for the intended application, accommodating frequency variations in the range of 20 MHz to 50 MHz commonly observed with magnetron sources. This broadband nature supports improved power matching and system stability. Moreover, the antenna structure is mechanically robust and designed for ease of precise fabrication, making it well-suited for practical deployment in high-power microwave processing environments.





Figure 2. (a) Waveguide and (b) Free Space 3D Electromagnetic Model, (c) Return Loss, (d) Axial Ratio and (e) Radiation Pattern for the Proposed Spiral Antenna.

3.1.2. Microwave Dryer and Pyrolysis Chamber:

The electromagnetic (EM) simulation model of the microwave processing chamber, integrated with the proposed circularly polarized spiral antenna, is presented in Figure 3. The chamber has internal dimensions of $385 \times 385 \times 390$ mm (L × W × H) and features a front-access door along with a top-mounted port designed to accommodate a quartz container. The chamber is optimized for dual functionality, enabling both microwave-assisted drying and pyrolysis of sludge samples. This flexibility is achieved through careful design and process control integration. To protect the magnetron and antenna assembly from backflow of moisture, vapor, or steam, the antenna is enclosed with a 10 mm thick polytetrafluoroethylene (PTFE) cover, which provides effective electrical insulation and chemical resistance while remaining transparent to microwaves.





Figure 3. 3D EM Model of the Microwave Dryer and Pyrolysis Chamber.

A microwave-transparent support structure is employed to hold the quartz container containing the wet sludge. During the drying process, the samples undergoes moisture loss, after which the same setup facilitates the pyrolysis of the dried material, utilizing microwave energy at the operating frequency of 2.45 GHz. Critical considerations were incorporated into the EM simulations to accurately model the dynamic behaviour of the samples during drying. As the sample dehydrates, its physical height, relative permittivity, and loss tangent vary significantly with changing moisture content, as detailed in Table 1. To capture this variability while ensuring computational feasibility, averaged dielectric property values across the expected moisture range were used for final simulation-based optimization.

3.1.3. EM – Simulation for the Drying Process:

For the optimization of the microwave chamber, a sample with an initial moisture content of 80% was selected from Table 1. This condition closely represents the targeted operational scenario for drying applications. The optimization focused particularly on adjusting the height of the metallic enclosure surrounding the antenna, while maintaining fixed dimensions for the quartz container, spiral antenna, and sample holder. The use of a pyramidal-shaped metallic enclosure is intended to enhance the antenna's directivity by concentrating microwave energy toward the sludge sample, thereby minimizing undesired dispersion within the chamber. This focused delivery is critical for improving heating efficiency and uniformity.



To support the simulations, average dielectric properties corresponding to the 80% moisture level were used, along with the appropriate sample height derived from Table 1. These parameters served as the basis for the electromagnetic optimization process. Simulation results confirmed effective power matching across all four configurations, with return losses exceeding 14 dB —indicating that more than 96% of the incident microwave power is accepted by the system (Figure 4). Furthermore, the spatial distribution of microwave power loss density within the sludge sample at constant input power levels is illustrated in Figures 5 through 8, highlighting energy absorption patterns under different enclosure height and moisture level configurations.



Figure 4. Return loss of the optimized chamber for the Sludge with (a) 80 %, (b) 60 %, (c) 40 % and (d) 20 % of Moisture respectively.



Figure 5. Microwave Power loss density in the sludge with 80 % of moisture.





Figure 6. Microwave Power loss density in the sludge with 60 % of moisture.



Figure 7. Microwave Power loss density in the sludge with 40 % of moisture.





Figure 8. Microwave Power loss density in the sludge with 20 % of moisture.

$$dp = \frac{\lambda_0}{2\pi \sqrt{2\epsilon \prime \left[\sqrt{1 + (\epsilon \prime \prime / \epsilon \prime)^2 - 1}\right]}} \tag{1}$$

As shown in Figure 5, despite the microwave energy being introduced from the bottom of the chamber, significant power loss occurs near both the bottom and top surfaces of the sludge sample—extending approximately 10 mm into the material from each end. This observation is based on a sample with an initial height of 75 mm and 80% moisture content from Table 1. The effective microwave penetration depth (dp), as described by Equation 1, is strongly influenced by the dielectric properties of the material —specifically, the relative permittivity and loss tangent —as well as the wavelength of the applied microwave signal. High moisture content generally results in higher dielectric losses, limiting the penetration depth and leading to non-uniform energy distribution. Further analysis of the simulation results (Figures 6 to 8) reveals that as the moisture content decreases, the penetration depth improves significantly. This results in more uniform power absorption and enhanced heating homogeneity throughout the sludge volume. Additionally, the reduction in sludge height, which occurs naturally during drying, contributes to improved field uniformity and more effective microwave energy utilization.

3.1.4. EM – Simulation for the Pyrolysis Process:

After optimizing the microwave drying chamber across a range of moisture levels and corresponding sludge heights, the same chamber configuration was employed to



evaluate microwave power matching and loss density distribution for a dried sample. This evaluation was based on representative dielectric properties and physical dimensions of the sludge at a reduced moisture content. For the dried sample with approximately 10% moisture content (from Table 1), the relative permittivity, loss tangent, and sample height were set to ranges of 5–10, 0.05–0.10, and 30 mm, respectively. Under these conditions, the system exhibited effective impedance matching, with a return loss of approximately 13.5 dB, as shown in Figure 9. This corresponds to a power acceptance of over 95%, indicating efficient energy coupling. Furthermore, the simulated microwave power loss density distribution demonstrated significantly improved penetration, with energy effectively absorbed across the full thickness of the sludge sample. This is illustrated in Figure 10, confirming uniform energy deposition and enhanced heating efficiency in the dried state.



Figure 9. Return loss of the optimized chamber for the Dried Sludge with 10 % of Moisture.





Figure 10. Microwave Power loss density in the dried sludge with 10 % of moisture.

3.3. Design and components

The conceptual and preliminary technical design of the microwave pyrolysis chamber for the FLEXBY project has been completed, incorporating simulation outcomes and operational process requirements. The configuration of the system is illustrated in Figure 11, showing the chamber layout and process flow, including essential piping, control, and monitoring components. We are currently finalizing the detailed design and initiating procurement of the mechanical and electronic parts required for the fabrication of the microwave pyrolysis system.





Figure 11. Microwave chamber schematics including main components.



All core components required for the chamber operation are listed in Figure 12, including pneumatic valves, sensors, measurement instruments, and safety systems. The system operates in two distinct modes: drying and pyrolysis.

A schematic figure (Figure 13) is included to illustrate the safety cabin and the microwave chamber housed within it.

Symbol	Function	Technical Data	Maker
$\mathbb{A}_{\mathbb{A}}$	1 pcs Pneumatik Magnetvalve for switch ON/OFF flow from preasure air	KN 05311HN 24V= Control supply : 24VDC	FESTO
	2 pcs pneumatic ball valves in the outlet to circulate the gas	24VDC actuator, unactuated closed Position feedback via Rotech Box DRZPF3SASAZ0, with 2 ind. switch P+F (SJ3,5-SN), cover with visual indicator OPEN-CLOSED, electrical feedback open/closed	Chemtech
	Intake compressed air ventilator	Vortex air compressor Possible choice : 2200W / 360mbar / 5400l/min 1500W / 220mbar / 3666l/min 750W / 220mbar / 2416l/min 370W / 160mbar / 1000//min	HPCONTROL (Polish company)
	XI80 IR Camera to observe the heating up and pyrolyse prozess of product in chamber	Optical resolution 80 x 80 pixels ; Spectral range 8 - 14 µm Temperature ranges 0 900 °C Frame rate 50 Hz Optics (FOV) 30° Focus Manual motor focus Optical resolution 190:1 Thermal sensitivity (NETD) 100 mK Accuracy ±2 °C or ±2 %, whichever is greater PC interfaces USB 2.0 / Ethernet (100 Mbit/s) / PoE / RS 4852) Analog output 4-20 mA	OPTRIS
	Temperature measurement in the air outlet pipe before and during the pyrolysis process (air temperature 900°C)	Thermoelement Typ K +900°C with transmitter 4-20mA	TC Direkt
	Hydrogen detector, for detecting hydrogen leakage within the chamber housing. If a leak is detected, the microwave power is switched off.	SI-200 Explosion-proof Diffusion Type Gas Detector	SENKO
	Rupture disk to protect the chamber from overpressure in the event of a product explosion	Operating pressure: max. 5bar Operating temperature : max 450°C	Rembe
	Measuring the air pressures in the air outlet pipe	Operating preasure 0-10bar	ACS
	Measuring and control the N2 inlet gas to chamber	N2 Gas flow meter 0,1 - 5l/min	Bronkhorst
	Measuring the humidty in Watersteam outlet	Humidity 0-100% +/-1% rf	EE-Electronic

Figure 12. Main components of the microwave pyrolysis machine, including heating units, sensors, flow controls, and safety systems integrated for efficient and safe operation.

3.4. Control, Regulation, and Safety Algorithms

The microwave pyrolysis system developed for the FLEXBY project features a robust integration of operator-defined controls, automated regulation algorithms, and layered



safety mechanisms. This ensures precise control of key process parameters while maintaining high safety standards throughout operation.

3.5.1 Key Experimental Parameters

The primary experimental variables controlled during the pyrolysis process are as follows:

• Moisture Content of Feedstock: Initial feed moisture is a critical parameter, typically ranging from ~90% down to 10–15% before pyrolysis. It is regulated in Drying Mode, which can be set by the operator based on time or real-time humidity data. A stepped humidity and temperature probe monitor the outlet gas, enabling indirect calibration of the feed's moisture content through weight-based measurements.

• **Microwave Power:** The microwave generator power is manually adjusted by the operator, with a maximum setting of 3 kW. This power level regulates the heating rate and determines the final temperature of the feedstock during pyrolysis.

• **Pyrolysis Duration:** The operator defines the processing time for once the feed temperature reaches the pyrolysis range (400–800 °C). For safety, if the feed reaches 700 °C, the maximum allowable pyrolysis duration is 20 minutes, after which the system automatically shuts down.

• **Temperature Regulation:** The feed temperature is continuously monitored using an infrared camera (Optris XI80). The outlet gas temperature is independently tracked with a K-type thermocouple, and is kept below 400 °C by modulating nitrogen flow, ensuring the protection of all downstream components.

Note: The analysis of biogas and the separation of gas and liquid fractions are managed externally by the project partner CSIC, which is responsible for post-reaction processing.

3.5.2 Reactor Control Algorithm

The process is structured into distinct, sequential stages with specific control logic:

• Manual Loading: The operator manually loads up to 2 kg of feedstock into a quartz glass reactor through the top opening. The reactor cap is securely closed to begin the process.



• **Drying Mode:** The system initiates drying by applying low-power microwave radiation, combined with the injection of air to prevent condensation inside the reactor. Drying can be controlled by:

- Operator-defined time, or
- \circ Target humidity, as measured by the humidity probe at the gas outlet.

• **Transition Phase:** Once drying is complete, air injection is fully stopped, the reactor is purged with nitrogen at ~2 L/min for at least 5-10 minutes to displace oxygen and establish an inert environment. After purging:

- $\circ~~N_2$ flow is reduced to ~200 mL/min to maintain inert conditions.
- The system switches to pyrolysis mode.

• **Pyrolysis Mode:** Microwave irradiation is initiated using 3 kW water-cooled magnetron heads, with power set by the operator. The outlet gas line is redirected at this stage to bypass the humidity sensor and allow connection to the biogas recovery system.

- Infrared temperature monitoring (XI80) ensures target feed temperatures (500-800 °C) are reached without exceeding limits.
- Exhaust gas temperature is controlled and maintained below 400 °C using adjustable nitrogen flow.

3.5.3 Safety Features

Safety is ensured through multiple protective systems integrated into both hardware and software:

• Enclosed Safety Cabin: The entire reactor assembly is housed within a dedicated safety cabin (Figure 13), providing:

- A physical barrier against heat and gas exposure.
- An exhaust port on top for connection to fume hoods or external ventilation.
- Isolation from external components for safer recovery system integration.

• Hydrogen Leak Detection: A hydrogen gas detector (SENKO SI-200) is installed near the reactor cap inside the cabin. In the event of H₂ detection, the system:

• Immediately shuts off microwave power



- Initiates a high-flow nitrogen purge to rapidly displace hydrogen and neutralize ignition risk.
- Pressure and Flow Safety: Additional integrated protections include:
 - A rupture disk to relieve overpressure.
 - Pneumatically actuated valves to isolate system sections.
 - Interlock systems that:
 - Cut power if water or nitrogen pressure drops below safe thresholds.
 - Trigger alarms to notify operators of hazardous conditions.

These features are designed to ensure safe operation in both routine and emergency scenarios. All controls and interlocks are fully integrated to work in coordination with the internal system logic.





Figure 13. Safety cabin enclosing the microwave chamber.



4. CONCLUSION

The simulation and design work presented in this report culminated in a robust and optimized prototype for a microwave-assisted pyrolysis reactor tailored to FLEXBY's goals of sustainable biofuel production from waste biomass. By leveraging detailed dielectric characterization and electromagnetic simulations, the project team successfully addressed key challenges associated with heating uniformity, energy efficiency, and system safety.

The dual-mode reactor—capable of both drying and pyrolysis within a single chamber—demonstrated excellent performance in terms of electromagnetic coupling, thermal response, and adaptability to feedstock variability. Safety-critical components and process control algorithms were integrated to ensure reliable operation under diverse conditions.

This deliverable concludes the simulation phase of the reactor development and paves the way for the construction, testing, and eventual deployment of the microwave pyrolysis system. The results affirm the feasibility of the FLEXBY approach and offer a replicable model for future bioenergy technologies.



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