

# I am CELISE

Sustainable production of  
Cellulose-based products and  
additives to be used in SMEs  
and rural areas

Deliverable D2.3. Smart  
systems in small  
biorefineries



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## **CELISE: Sustainable production of Cellulose-based products and additives to be used in SMEs and rural areas**

### **Deliverable D2.3. Smart systems in small biorefineries**

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### 3. LIST OF ABBREVIATIONS

*Table 2. List of abbreviations*

<b>Acronym</b>	<b>Definition</b>
ANN	Artificial Neural Network
CA	Consortium Agreement
CT	Coordination Team
D	Deliverable



### 4. INTRODUCTION

#### 4.1. General purpose of the document

This document provides an overview of the activities carried out under Deliverable D2.3, which focuses on the development, integration, and validation of smart-system approaches in small biorefineries, with particular emphasis on artificial neural network modelling. As Deliverable D2.3 partially overlaps with the methodological scope of D2.2—especially in relation to the use of ANN-based tools for process simulation and optimisation—this document summarises and extends the relevant material to ensure consistency across the work performed within WP2.

The present deliverable consolidates the results connected to the application of intelligent computational methods to biomass pre-treatment processes, aiming to advance data-driven and adaptive decision-support tools for small-scale biorefinery environments. The activities reported here build upon the ANN modelling framework described in D2.2, while incorporating the specific contributions and experimental contexts associated with the mobility periods and research tasks assigned to D2.3.

#### 4.2. Role and contribution from partners

Deliverable D2.3 forms part of the activities conducted within Work Package 2 (WP2). The tasks carried out in this deliverable have been primarily performed through the collaboration of four project partners: (i) UPM – Universidad Politécnica de Madrid, (ii) AUTH – Aristotle University of Thessaloniki, (iii) ECORESOUR (Ecoresources, IKA), and (iv) Latitud – Fundación Laboratorio Tecnológico del Uruguay.

These partners have contributed to the development of artificial neural network models, data processing workflows, process simulation routines, and analytical tasks related to the assessment of biomass pre-treatment performance. The mobility periods hosted by these institutions enabled the generation of primary data, the refinement of model architectures, and the integration of ANN-based tools into the broader conceptual framework of smart small biorefineries.

While D2.2 brought together a larger consortium of institutions involved in modelling, simulation, techno-economic assessment and life cycle analysis, the scope of D2.3 is more focused, reflecting the specific contributions of UPM, AUTH, ECORES, and Latitud to the methodological development and validation activities required for this deliverable.



## 5. SMART SYSTEMS IN SMALL BIOREFINERIES

### **(Based on Deliverable D2.2: Mathematical tools in small biorefineries: artificial neural network models, simulation and optimization and LCA)**

This section provides a consolidated summary on the role of smart systems in small biorefineries, derived from the content presented in Deliverable D2.2. Mathematical tools in small biorefineries: artificial neural network models, simulation and optimization and LCA, specifically from the part devoted to artificial neural network (ANN) modelling. As the present deliverable addresses related methodological aspects, and there is partial overlap with D2.2, the purpose of this summary is to ensure consistency across project outputs and to provide a coherent integration of the main findings relevant to data-driven and intelligent biorefinery operation.

Deliverable D2.2 demonstrates that artificial neural networks constitute a key enabling technology for the development of smart biorefineries, particularly within the context of small-scale facilities operating under constraints related to raw material variability, reduced process integration, and limited experimental capacity. In such settings, conventional mechanistic models often fail to capture the nonlinear and feedstock-dependent behaviour that characterizes lignocellulosic pretreatment processes. To address this limitation, D2.2 introduces ANN-based modelling approaches capable of learning and generalizing complex multivariate relationships from empirical data.

The deliverable reports the development and implementation of multilayer perceptron (MLP) architectures, supported by data preprocessing (normalisation, dimensionality reduction through principal component analysis) and advanced training strategies (resilient backpropagation, validation-based early stopping, and bootstrap-derived ensemble modelling). These methodological elements collectively ensure model robustness and reduce overfitting risks, which is particularly relevant given the restricted availability of primary data commonly encountered in small biorefinery operations.

The application of ANNs to steam explosion pretreatment is presented as a representative example. The model links initial biomass composition—encompassing extractives, structural carbohydrates, lignin fractions, acetyl groups and ash content—to pretreatment conditions (temperature and residence time) and final compositional outcomes (cellulose, hemicellulose and lignin). The resulting ANN models exhibit high predictive performance, explaining over 75% of the variance in all output fractions across several biomass types (e.g. sugarcane bagasse, Eucalyptus spp., pine residues and Arundo donax). These findings confirm that ANN-based simulators are capable of handling the heterogeneity typical of decentralized biomass supply chains. Moreover, the deliverable presents optimisation surfaces generated from the trained models, which allow identification of operating windows that maximise specific product fractions. For instance, high-severity conditions (200 °C, 20 min) favour cellulose and lignin yields, whereas hemicellulose is preserved under milder conditions (170 °C, 5 min). Such outputs provide actionable guidance for small biorefineries seeking to adapt process severity to specific valorisation pathways while minimising trial-and-error experimentation.

A second ANN-based smart system is developed for hydrothermal and dilute-acid pretreatment. In this case, limited dataset size is mitigated through bootstrap-based data augmentation, ensuring that the ANN can be trained without compromising predictive accuracy. The model is applied to simulate glucan recovery as a function of biomass composition and pretreatment conditions, with optimal glucan retention being observed at comparatively mild temperatures



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and short reaction times. Additionally, the distribution of simulated values is examined, enabling an uncertainty-aware interpretation of model outputs. This approach demonstrates the feasibility of employing ANN-based tools in data-constrained contexts, which are characteristic of small-scale biorefineries.



### 6. CONCLUSIONS

Artificial neural networks are core components of smart, data-driven process management frameworks for small biorefineries. Their ability to simulate process performance, evaluate alternative operating conditions, and support optimisation renders them highly suitable for facilities where operational flexibility, rapid scenario analysis and efficient resource use are essential. The ANN-based mathematical tools described in D2.2 contribute directly to the project's overarching objective of enabling intelligent, adaptable and efficient biorefinery systems through the integration of advanced computational methods.