Biodegradation Prediction and Modelling for Decision Support

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Abstract: In this paper we describe the functionality of a decision support modelling approach to select appropriate biomaterial blends depending on their mechanical/chemical properties on the one hand, and their biodegradation behaviour, on the other. Firstly, a Case Based Reasoning (CBR) approach is applied to predict expected biodegradation behaviour over time, based on historical examples and using a weighted distance metric on the material properties in order to calculate the trend curve of the new case. Secondly, a Multi-Agent System (MAS) is applied to dynamically simulate the biodegradation curve, in which the two main agents, bacteria and plastic, interact to reproduce the biodegradation kinetics over time. The results of the interpolation are very promising with a good approximation to the real curve time series and % biodegradation, and the Multi-Agent System successfully simulates the different trend curves over time. The system has been confirmed as useful by materials expert end-users, who participated in the project, in order to evaluate *a priori* new blends "in silico", and identify and select the most promising, before conducting the long duration biodegradation experiments in the real environment.

1 INTRODUCTION

Developing biodegradable materials which are fit for purpose in the future circular economy is a critical task if we wish to make the transition from fossil fuel plastics. However, finding an equilibrium between mechanical properties of the different potential bio-material blends and their biodegradation requirements can be a complex, trial and error, and lengthy process (due to the long experimental time required for biodegradation testing).

Hence, it is of great interest to be able to accurately model and predict the biodegradation process of potential material blends, in order to focus on the most promising and reduce experimental testing time.

In this paper, we show that Case Based Reasoning and Multi-Agent System modelling approaches can be useful to generate the biodegradation prediction of a new blend based on material properties, and simulate the corresponding biodegradation curve. The results are very promising, although on a limited set of cases, for predicting best and worst performers.

First, the CBR obtains the closest historical cases to a new one, interpolates and expected trend curve, and then passes this information to the MAS to simulate in a kinetic and stochastic solution space.

The motivation of using CBR and MAS for predicting and simulating the biodegradation process, comes from the shortcomings of existing approaches,

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such as the need for complex representations of large amounts of low level chemical knowledge, and the lack of representation of stochastic and kinetic features.

The system is defined "as a service", where material designers and testers provide the material characteristics and the system returns the predicted biodegradation behaviour (curve over time).

The paper is organized as follows: in Section 2 related work is presented, in Section 3 the data used and pre-processing is summarized, in Section 4 the Case Based Reasoning processing and matching approach is described with examples, in Section 5 the Multi-Agent System based simulation is described and Section 6 summarizes the work. Also, a Dynamic System Model definition of the biodegradation process is given in the Annex.

2 RELATED WORK AND BACKGROUND

There is an extensive literature of chemical based biodegradation modelling, using traditional statistical techniques together with detailed chemical knowledge (Pavan and Worth, 2006;2008), as well as more recent approaches based on kinetic modelling(Farzi et al., 2019; Sonwani et al., 2020; Sable et al., 2019). However, data modelling using a simple set of descriptive parameters including chemical and mechanical properties and using artificial intelligence techniques is more difficult to find in the literature. Hence, this is one of the key motivations and advantages for our current work.

Purely chemical based approaches for the biodegradability of material require highly specialized parameterisations, such as in (Alalayah, 2017) (Dragomir et al, 2021), which require deep chemical knowledge.

Furthermore, sets of ordinary differential equations (ODEs) have limitations when representing problems which involve spatial interactions or emerging properties (Borshchev and Filippov, 2004), and present difficulties for embodying emergent and stochastic behaviour. (Pavan and Worth, 2006;2008) consider QSAR (Quantitative Structure-Activity Relationship) which is an important family of models for chemical modelling. QSARs are mathematical models that can be used to predict different properties of compounds from the knowledge of their chemical structure.

In terms of AI techniques applied specifically to biodegradation modelling, neural networks and rule induction are two examples. (Gamberger, et al., 1996) used a rule induction technique and chemical feature sets as inputs. The biodegradation data from both data-bases are discrete values, i.e. those chemicals are classified as biodegradable or non-biodegradable. The work of (Baker et al., 2004), uses rule induction and as input includes complex low level chemical information. Binary output variables are assigned to each chemical with a 1 for fast biodegradability and 0 for slow biodegradability. (Arranz, et al., 2008) used neural networks to model biodegradation processes, requiring a high number of samples to train the network. Note that in the case of (Gamberger et al., 1996) and (Baker et al., 2004), their models are limited to producing a binary classification as output. In contrast, our solution produces the trend curve with quantified values for % biodegradation and time.

In their review paper, (Baker et al., 2004) indicated the use of multiple linear regression and artificial neural networks, Partial least squares discriminant analysis and Inductive machine learning (rule based), among others, however the focus was on a lower level chemical analysis. Also from (Baker et al., 2004), a Knowledge-based learning system was described as a method using machine learning techniques to determine relevant descriptors mathematically from data on activity and basic chemical structure. Furthermore, Multi-Agent based systems (MAS) (Ferber and Weiss, 1999) and Dynamic System Models (DSM) (Radzicki and Taylor, 2008) have been used for stochastic system modelling in different fields. As recent examples, (Nettleton et al., 2020) and (Estivill-Castro et al., 2021) have applied and contrasted the utility of MAS and DSM for clinical applications, simulating multiple trend curves over time for modelling complex kinetic interactions and behaviours between the human immune system and cancer cells.

The case for using MAS in preference to mathematical models and DSMs is supported by the ability of the former to more easily simulate kinetic and stochastic behaviour, as well as being data driven so requiring less theoretical know-how to be pre-defined.

The current work takes (Nettleton et al., 2020) and (Estivill-Castro et al., 2021) as starting point to apply the MAS approach to the novel application of bioplastic blend biodegradation over time. Case Based Reasoning (CBR) (Aamodt and Plaza, 1994) is also an approach taken from artificial intelligence which essentially uses a set of historical cases as a reference in order to find the closest match to a new case. In the current work we use CBR as pre-processing for the MAS, in order to match the material properties of a new blend to find the closest

historical blends, and hence their corresponding biodegradation trend curves.

The EU Horizon 2020 project Biontop, of which the current work forms a part, is aimed at developing novel packaging films and textiles with tailored end of life and performance based on bio-based polymers. In the framework of the project bioplastics blends based on biobased and industrially compostable Poly(lactic acid) (PLA) were considered (Narancic et al., 2018). The blending with other bio-polyesters resulted successful for modulating the mechanical properties of this polymer in a wide range of values (Aliotta et al., 2021;2021). One key aim of the project is to find bioplastics which are 'home-compostable', which means they are biodegradable at a lower temperature and in milder conditions than those typical of 'industrial composting'.

Hence, the biodegradation testing of blends was performed for home-composting conditions, executed according to ISO 14855 but at ambient temperature (28°C). The tests were carried out using pellets produced by twin screw extrusion in a Comac EBC 25 HT extruder (Comac, Milan, Italy).

In the Appendix can be found a dynamic system model (DSM) simplified representation of the bioreactor set-up. A DSM typically consists of a stock and flow diagram (Figure 7), a set of differential equations to represent the behaviour of the stocks over time (Table 6), a set of algebraic equations to define the flows (Table 7), and a set of control parameters used by the system (Table 8). In Figure 7, five stocks are defined: bioplastic, compost, Reactor, O_2 and CO_2. The flow on the top right indicates the bioplastic formulation (blend) which is input at the process start as a batch. The flows below are O_2 which oxygenated the Reactor and compost, which is input at the process start as a batch and is the source of the bacteria. On the right is the CO_2 stock produced as output (by the biodegradation process) inside the Reactor stock which is located in the middle. The degree is biodegradation is quantified from the CO_2 readings.

3 DATA AND PRE-PROCESSING

The data used for prediction and modelling is based on the materials properties (chemical and mechanical) as shown in Table 1, and the biodegradation results of each material, as shown in Table 2 and Figures 1 and 2. Eight material blends were used for biodegradation testing, as part of the Biontop project (see background Section). Note that for confidentiality reasons and intellectual property protection of the Biontop project, the data has been normalized or rescaled, and the material names anonymized. However, this has been done in a way so as to maintain the relative values and interpretability of the data with the results.

Table 1 shows a summary of the chemical and mechanical properties of the eight main bioplastic materials, named as blends 1 to 8. For confidentiality reasons, all material property values are normalized in a range between 0.5 and 1.5, and the biodegradation times are scaled between 0 and 1. It can be seen that in terms of chemical properties, blend 7 has a low molecular weight and medium polarity and crystallinity; in terms of mechanical properties, it has a low Young's Modulus, a low elongation at break and a high tensile strength.

Table 2 shows a summary of the biodegradation results for the eight material blends whose characteristics were given in Table 1. It can be seen that blend 7 gives the best biodegradation results, reaching 100% biodegradation in a scaled time of 0.6. On the other extreme, the blend 5 material gives the worst biodegradation results, achieving only 1.2% biodegradation in a scaled time of 1.0 (highest value).

From the material characteristics of Table 1 and the biodegradation results of Table 2, a strong correlation is evident between the two. For example, a low molecular weight and high crystallinity give a propensity for the material to biodegrade.

We note that only eight cases (i.e. blends) were available from the Biontop project with their full material properties data and biodegradation results. However, they were chosen, by the materials experts involved in the project, to cover a realistic and representative distribution of scenarios from good biodegradation (blends 4 and 6 to 8), medium (blend 3) and poor (blends 1, 2 and 5).

Figures 1 and 2 show all the biodegradation trend curves for the eight blends which were empirically tested.

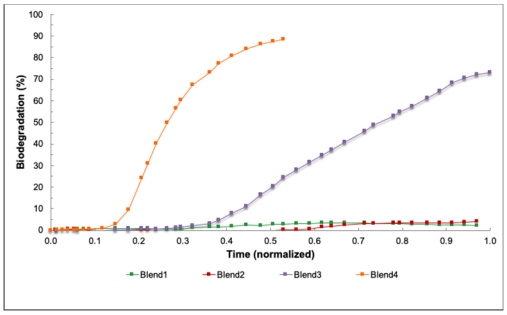

Figure 1: Biodegradation curves for blends 1 to 4.

Table 1: Chemical and mechanical properties of blends 1 to 8*.

Chemical and Mechanical Properties	Blend1	Blend2	Blend3	Blend4	Blend5	Blend6	Blend7	Blend8
Polarity	0.7	0.7	1.4	1.5	0.8	1.3	1.2	1.1
Molecular weights	1.5	1.4	0.9	0.7	1.3	0.6	0.6	0.5
Crystallinity	1.5	1.2	0.9	0.7	1.5	0.7	0.8	0.5
MFR	0.5	0.6	0.6	0.7	1.3	1.4	1.4	1.5
Impact strength	0.7	0.8	0.9	1.5	0.7	1.4	1.4	1.5
Tensile strength	1.2	1.1	0.5	0.9	1.5	0.5	0.6	0.8
Young's Modulus	1.5	1.3	1.0	0.8	1.5	0.5	0.5	0.6
Elongation at break	0.5	0.7	1.1	1.5	0.5	1.2	1.2	1.2

*All values are normalized to a range between 0.5 and 1.5.

Table 2: Biodegradation results of blends 1 to 8*.

Biodegradation Criteria	Blend1	Blend2	Blend3	Blend4	Blend5	Blend6	Blend7	Blend8
Time to 50%			0.8	0.3		0.2	0.2	0.2
Time to 100% or MAX	0.6	1.0	1.0	0.5	1.0	0.6	0.6	0.7
Max%	3.5	4.2	73	88	1.2	97.7	100	90.3
Rank biodegradability	6	7	5	4	8	2	1	3

*All values (except max%) are scaled to a range between 0 and 1.0.

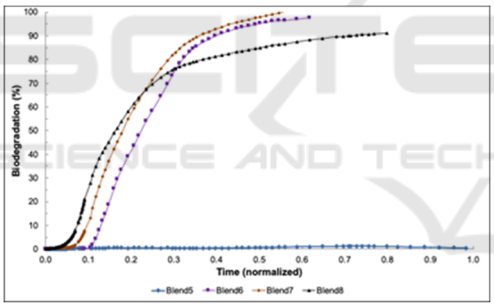

Figure 2: Biodegradation curves for blends 5 to 8.

4 CASE BASED MATCHING

In this section we explain how the Case Based Matching approach with an appropriate distance metric, is applied to the material properties and biodegradation data in order to predict the biodegradation of new blends.

4.1 Modus Operandi and Example Applying CBM to Material Properties and Blend Biodegradation Data

The data processing of the CBM approach has the following four steps, with reference to Table 3, Figure 3 and Equation (1): **(i)** choose one blend as "new blend" (e.g. blend8); **(ii)** calculate "distance" between new blend and all remaining historical blends using only material properties data (i.e. only a priori information); **(iii)** identify two "closest" historical blends in terms of distance (e.g. blends 6 and 7); **(iv)** use the two "closest" historical blends to interpolate curve of "new blend" (Figure 3).

The distance D is calculated by applying a Euclidean metric to the respective material properties (Table 1) and summing over n, the number of properties, which are previously normalized and have equal weighting:

$$\mathrm{D} = \sum_{i=1}^{n} |(p_{i1} - p_{i2})| \quad (1)$$

where p_{i1} is property i of material 1 and p_{i2} is property i of material 2.

Table 3 shows the seven blends used as the historical case base and blend 8 considered as a "new" blend (but whose biodegradation results are known). Blends 6 and 7 are found to be the "closest" to blend 8 (from all 7 available historical blends) using the distance metric calculation. This gives a distance of 0.7 and 0.6, respectively for blends 6 and 7.

Table 3: Blends selected as historical examples and new blend.

Historical examples	Distance to Blend 8
Blend1	1.5
Blend2	1.5
Blend3	1.0
Blend4	0.8
Blend5	1.5
Blend6	0.7
Blend7	0.6

Now, using the curve points y_1 and y_2 of existing blends 6 and 7, respectively, the corresponding curve point approximation y' for the new blend is obtained: first the distances of Table 3 are normalized and then the two smallest values used as weights w_1 and w_2 to interpolate. From this, the polynomial equation is estimated which best fits the curves Y_1 and Y_2 and the individual points y' (% biodegradation over time) are calculated thus:

$$\forall y > 0, w \in [0..1]$$
$$y'_1 = y_1 \times w_1$$
$$y'_2 = y_2 \times w_2 \quad (2)$$
$$y' = y'_1 + y'_2$$

Hence, the overall result of the case matching of a new blend with historical blends, is to obtain a new interpolated biodegradation trend curve over time. In Figure 3 it is shown that blends 6 and 7 are identified as the closest blends to the "new" blend 8, based on chemical and mechanical properties. Also in Figure 3 is seen how the blend 8 curve is interpolated from the curves of blends 6 and 7, using the weighted distance metric (Equation 2) to generate the points. In the case of blend 8, the fit of the interpolated curve to the real blend 8 curve is relatively lower (0.75, see Table 4).

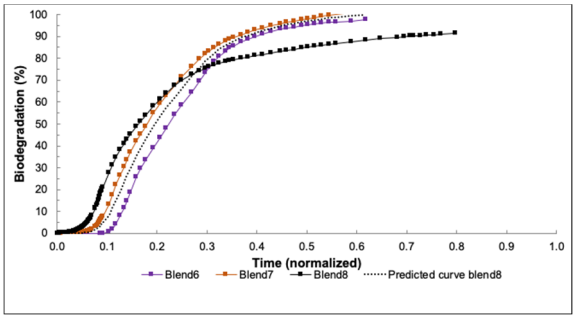

Figure 3: Closest historical curves and new curve interpolation.

This is because the trend of the real curve for blend 8 flattens out from time 0.3 onwards, diverging from the trends of blend curves 6 and 7. However, at this point it has already reached almost 80% biodegradation (Figure 2).

4.2 Results of Applying CBM to Predict Biodegradation Curve of Blends

The process described in Section 4.1 with blend 8 as the "new blend", was repeated for blends 1 to 7. Table 4 shows the results of comparing the trend curves predicted by CBM with the real curves, for each of the blends. It can be seen that all the R^2 values of the matches were over 0.81, with the exception of blends 3 and 8, with R^2 values of 0.68 and 0.75, respectively. The lower performance for blends 3 and 8 was expected as they have intermediate biodegradation performance with respect to the best blends for biodegradation and the worst ones (see Figures 1 and 2). In summary, estimated blend curves 1, 2 and 5 are fitting closely together, also blends 4, 6 and 7, while blends 3 and 8 are relative 'outliers'. This is supported by the $R^{2'}$ values shown in Table 4.

Table 4: Matching of simulated data trend curve (simulated data) with real trend curve - R^2 value.

Composition /Blend	Trend curve (simulated data) vs trend curve (real data) – R^2 value
Blend1	0.9440
Blend2	0.9379
Blend3	0.6830
Blend4	0.8174
Blend5	0.9373
Blend6	0.9002
Blend7	0.8907
Blend8	0.7506

Furthermore, two aspects are of interest to the material experts: what is the % degradation at time 0.6 (or less) and how long does it take to reach a given biodegradation %. In general, the estimated curves provide a good approximation of this information. Note that for blends 3 and 8, the matching is with curves of shorter duration (0.6) and so the estimated curves get truncated at this limit. Hence, in conclusion, special attention has to be made to defining similar experimental conditions (time duration) for blend testing and having sub-groups of similar blends for comparison proximity. The accuracy for % at time 0.6 was generally within 15% for blends 3 and 8, 10% for blends 4, 6 and 7, and within 5% for blends 1,2 and 5. For the former, this was more dependent on the cut-off time of the closest blends chosen.

5 MULTI-AGENT SIMULATION

In this section we use a Multi-Agent System (MAS) to simulate the blend biodegradation behaviour, based on the trend curves. This requires the adjustment of the MAS control parameters (biodegrade chance, biodegrade distance, detect distance, speed) which act in a 2D solution space during the process.

As a starting point, the control parameters are assigned as a generic "predator-prey" model (Bădică et al., 2018; Karsai et al., 2016) which is interpreted in the current context as a kinetic model where the predator is the bacteria and the prey is the plastic. Furthermore, a plastic agent remains fairly static whereas a bacterium is more mobile, performing a random walk at a given "speed" (SP) until a plastic agent comes within its "detect distance" (DD). Once this happens the bacteria agent moves directly towards the plastic agent until it reaches the "biodegrade distance" (BD), and then, depending on the "biodegrade chance" (BC), it will biodegrade the plastic agent (i.e. the plastic agent is consumed and disappears). This apparently simple individual behaviour can give rise to a complex collective system, and more advanced interaction rules can be programmed into the agents. Figure 4 illustrates the concept of the two dimensional state space and respective action distances between the agents.

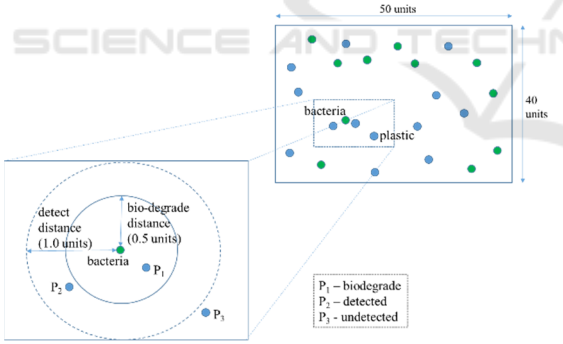

Figure 4: State space definition for agent interactions.

5.1 Modus Operandi

It is recalled that the CBM processing approach applied in Section 4 obtains the polynomial trend curve for the new blend. Now, we provide the trend curve (polynomial equation) to the MAS, and as it runs the agent system control parameters adapt in order to keep the population (of plastic) as close as possible to the trend curve. A weighting is also used for each control parameter.

The process is repeated ad-hoc for several trend curves, until a historical of results (trend curves with their corresponding agent control parameters) is accumulated. Once sufficient historical examples are available, the agent control parameter initial values and weighting can be automatically estimated for a new trend curve, without having to perform ad-hoc testing (thus significantly reducing the testing and refinement cycles to obtain the settings).

The control parameters are updated as follows: let P_1 be the expected plastic biodegradation percentage calculated from the trend curve and P_2 the current plastic agent population percentage in the MAS. Then, the percentage difference P_Δ between the two will be:

$$P_\Delta = \frac{(P_1 - P_2)}{P_1} \quad .$$

Next, a multiplier coefficient is defined as:

$$mu = 1.0 + P_\Delta$$

Then, the update rules are defined as:

$$BC = min(1, BC \times mu)$$

$$BD = BD \times min(1, mu)$$

$$SP = SP \times mu$$

$$DD = DD \times mu \qquad (3)$$

where BC = biodegrade chance, BD = biodegrade distance, SP = speed and DD = detect distance.

5.2 Results of Applying MAS to Blend Biodegradation Data

Figure 5 shows the results for the agent simulation processing the blend 3 trend curve. On the left are the Multi-Agent user interface screens where the blue dots represent the "plastic agents" and the green dots represent the "bacteria agents". The initial state is seen on the top left (with an equal amount of blue and green dots) and the final state is on the bottom left (with many more green and less blue). That is, the biodegradation process has worked, the bacteria have biodegraded the plastic. The right side of Figure 5 shows the corresponding simulation over time (accelerated time which processes a long time period in just a few minutes). On the top right is the real biodegradation curve for the new blend 3, and on the bottom right (green line) is the Multi-Agent simulation result. It can be seen that the simulated curve (bottom right) is a good approximation of the real curve (top right) in final percentage reached (70%) and normalized time duration of 1.0, as well as the gradient and general trend of the curve.

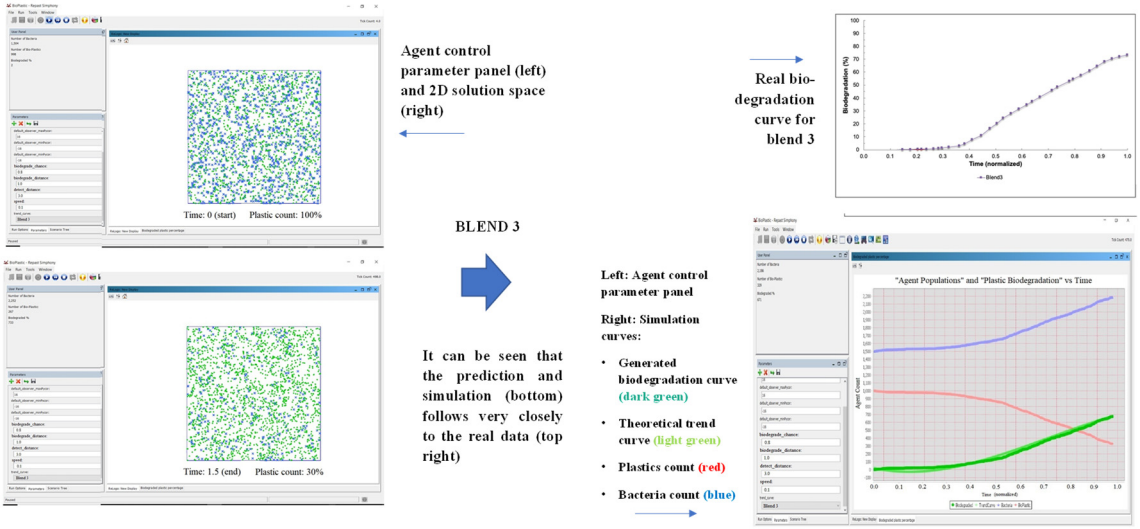

Figure 5: Agent simulation (Blend 3).

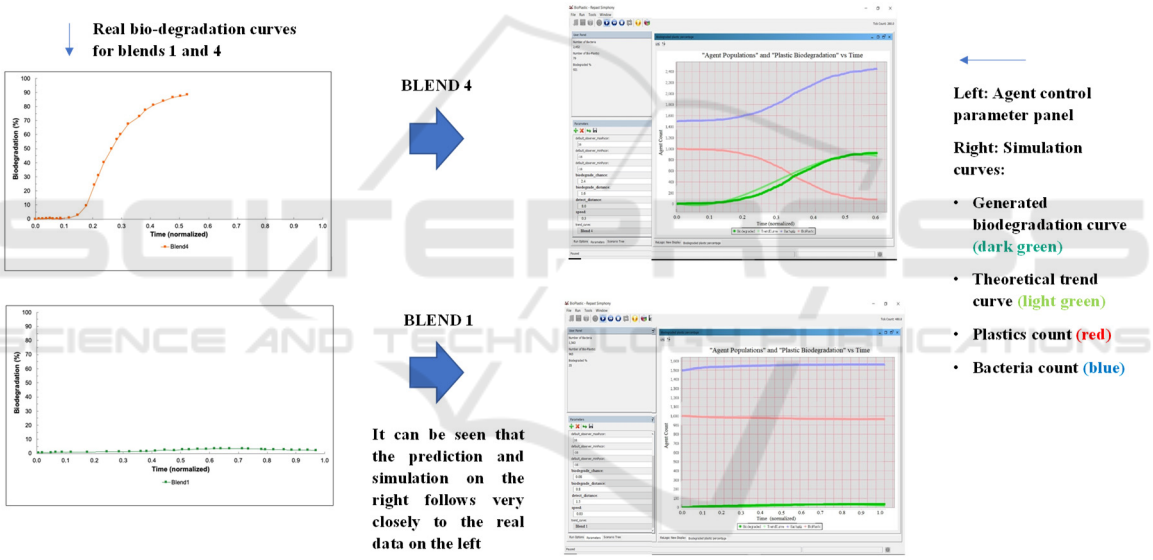

Figure 6: Agent simulation (Blends 1 and 4).

Having successfully simulated blend 3, we now perform the same process for blends 1 and 4, as shown in Figure 6. These blends represent the best performer and the worst, respectively, in terms of biodegradation behaviour. On the left of Figure 6 are shown the real trend curves over time, where it can be seen that blend 4 reaches 90% biodegradation with a normalized time duration of 0.6, whereas the blend 1 only achieves a max. of 5% with a normalized time duration of 0.8. On the right of Figure 6 it can be seen that the Multi-Agent system successfully models both trend curves over time and % end point, with the green curve of blend 4 shown on the top right and the green curve of blend 1 shown on the bottom right.

Table 5: Multi-agent system control parameters for three different biodegradation simulations*.

	Bio-degrade chance	Bio-degrade distance	Detect distance	Speed
Blend 1	0.08	0.8	1.5	0.03
Blend 3	0.8	1.0	3.0	0.1
Blend 4	2.4	1.6	8.0	0.3

*Values have been anonymized while maintaining their relative magnitudes.

Table 5 shows the control parameters used for the simulations of biodegradation for blends 1, 3 and 4, which are depicted in Figures 5 and 6. The four control parameters are given which relate to the bacteria and plastic agents: distance in which a bacteria agent can detect and “biodegrade” a plastic

agent, and the speed of movement for the bacteria agent.

It can be seen that blend 4, which has one of the best biodegradation behaviours (in terms of time and %, see Table 2) has the highest relative values for all four control parameters. On the other hand, blend 1, which has the worst biodegradation, has the lowest values, also for all four control parameters. This is explained by the degree of "excitation" of the system necessary in order to replicate the biodegradation curves (see Figures 5 and 6) in terms of agent populations. It could be interpreted as a degree of "kinetic energy" of the bacteria and the plastic. Blend 3, which displays an intermediate level of biodegradation, shows intermediate values for its control parameters, relative to blends 1 and 4, however the relation between the control parameters of the blends is non-linear. For example, the "biodegrade chance" for blend 1 is 10 times less than blend 3, whereas the "biodegrade chance" of blend 4 is only three times that of blend 3. It can be interpreted also in terms of the "distance" between the trend curves (Figures 5 and 6) and also between the respective material properties (Table 1).

In each case, the MAS control parameters have been optimized manually for each blend. However, as we progressively obtain a set of historical settings, they can be used to approximate settings (at least as an initial starting point) for new blends, in a similar way to the CBR, based on some distance function related to the material properties.

6 CONCLUSIONS

In this paper we have explained how a Case Based Reasoning (CBR) approach can be used to predict a biodegradation trend curve over time and how a Multi-Agent System can be applied to simulating the biodegradation process.

The CBR approach has been demonstrated to be able to generate a biodegradation prediction and trend curve for a blend, which is a good fit to real data, using the chemical/mechanical properties for matching closest historical cases, which is calculated using a weighted distance function. The results in Table 4 show all R^2 fitting values of predicted vs real curves to be over 0.81, with the exception of outlier blends 3 and 8 (refer to Section 4.2 for explanation).

Furthermore, we have demonstrated how a MAS can be used to simulate the corresponding biodegradation curves, with dynamic weighted MAS control parameter calculation (Table 5) tuned for each trend curve.

The results are clearly promising and verified as useful by the materials experts who design blends which must comply with given chemical and mechanical properties on the one hand, and biodegradation characteristics on the other.

The choice of material properties provided a strong set of descriptors with a good correlation between chemical and mechanical properties and their biodegradation behaviour. However, in order to obtain a good predictive capability from the CBR, a combination of a non-trivial weighted distance calculation and an interpolation method were necessary. In the case of the MAS, the real-time control parameter optimization also used a set of non-trivial updating formulas including weighting factors. Overall, the approaches appear to offer promising solutions for a variety of bioplastic blends, for their biodegradation trend prediction and dynamic simulation, respectively.

Also, the MAS offers a simulation solution which is relatively easy to implement and calibrate, in contrast with DSM and mathematical modelling approaches. Furthermore, the MAS is able to embody stochastic and noisy features present in real systems,

As future work, as part of the ongoing Biontop project, we expect to incorporate new blends into the modelling. Also, we plan to develop further the MAS modelling, by improving the induction of the MAS control parameters from the material properties, thus generating the trend curve automatically. Furthermore, the MAS control parameters, which were initially optimized manually for the different blends, can be used to find settings for new blends, in a similar way to the CBR approach.

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APPENDIX

The following defines the Dynamic System Model representation of the biodegradation process. Figure 7 shows the overall schema of stocks and flows, Tables 6 and 7 show the differential and algebraic equations, respectively, and Table 8 shows the systemic variables and parameters. See Section 2 of the paper for further explanation.

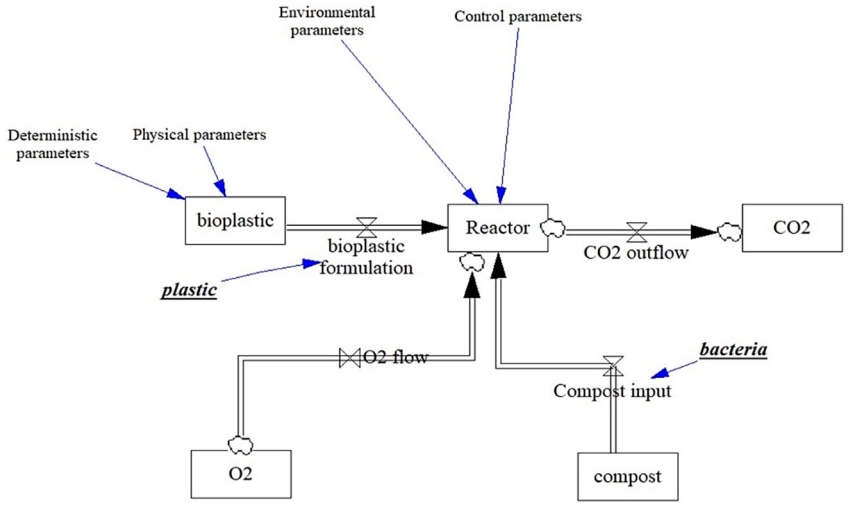

Figure 7: Stocks and Flows.

Table 6: Differential Equations.

Equation no.	Stock	Differential equations	Units
1	Reactor	$\frac{dBioplastic(t)}{dt} + \frac{dCompost(t)}{dt} = reactor(t)$	kg/d
2	Bioplastic	$\frac{dBioplastic(t)}{dt} = bioplastic(t)$	kg/d
3	Compost	$\frac{dCompost(t)}{dt} =$ compost(t)	kg/d
4	Bacteria	$\frac{dbacteria(t)}{dt} =$ bacteria(t)	%
5	CO2	$\frac{dCO2(t)}{dt} = CO2(t)$	cm^3/h
6	O2	$\frac{dO2(t)}{dt} = O2(t)$	cm^3/h

Table 7: Algebraic Equations.

Equation no.	Flow	Algebraic equations	Units
1	Biodecomposition material	Biodegradation material(t) = bioplastic(t) + compost(t) + O2(t) – CO2(t)	kg/h
2	O2	O2(t) = O2	cm^3/h
3	CO2	CO2(t) = CO2	cm^3/h
Quality criteria			
4	Quality 1	Decomposition time	days
5	Quality 2	% decomposition* achieved (absolute and/or relative)	%
6	Quality 3	Time to reach a target decomposition*	days

Table 8: Systemic variables and parameters.

Nº.	Parameter	Value(s)	Units
1	Amount of bioplastic	c_1	kg
2	Amount of compost	c_2	kg
3	Bioplastic formulation	c_3	-
4	Average absolute humidity	c_4	g/M^3
5	O2	c_5	cm^3/h
6	CO2	c_6	cm^3/h
7	Cut off time	c_7	days
8	Cut off %	c_8	%
9	Mechanical properties of bioplastics	p_1 , p_n	
10	Chemical properties of bioplastics (DETERMINISTIC)	d_1 , d_n	
11	Composting conditions (ENVIRONMENTAL, less DETERMINISTIC)	e_1 , e_n	