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System modelling of hydrolytic degradation in cellulose acetate artefacts

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BACKGROUND

With industrial-scale production starting in the early 20th century, cellulose acetate is one of the oldest types of plastic materials [1]. The semi-synthetic polymer is found in many modern collections, from historical objects to contemporary sculptures.

With short service lifetimes, an unpredictable rate of degradation, and emissions of damaging volatile organics compounds (VOCs), cellulose acetate is considered a high-risk material by conservation professionals [2]. The main degradation processes have been studied in isolation, but it has not been established how these interact in a complex system [3]. This makes it difficult to predict the impact of environmental factors such as temperature or relative humidity, or to assess if inherent properties of the object such as composition or thickness put it greater risk for degradation.

Hydrolysis reactions (deacetylation and glycoside bond cleavage) are known to play a major role in the degradation of the polymer [2]. This research aims to develop an equation-based model which predicts the spatial and temporal changes in composition due to hydrolytic degradation in cellulose acetate.

RESEARCH QUESTIONS

- ❖ How can the relevant physical and chemical processes be described mathematically and integrated into a system model?
- ❖ Based on this model, how do environmental and inherent factors affect the hydrolytic degradation of cellulose acetate?

METHODS

A **model** is a representation of a system which links inputs to outputs. Modelling work will take four steps:

1. **Descriptive model**: Distinctive processes are considered as acting upon a single system (see Fig. 1). These processes are included because they affect the concentrations of the chemical species involved in hydrolysis reaction. All the processes may be individually described by established mathematical models obtained from the literature. These are combined into a system of equations, mainly partial or ordinary differential equations.
2. **Predictive model**: The system of equations is solved using numerical methods and suitable software, for example MATLAB. Simulations may be run with different sets of input values and predict outputs as time- and space-dependent concentrations of chemical components (see Fig. 2).
3. **Model validation/optimisation**: Model predictions are compared against real data from the literature or from experiments. This is used to refine the model and make changes so that model predictions become more accurate.
4. **Sensitivity analysis**: Using the validated model, the effect of changes in inputs on outputs will be analysed quantitatively. The sensitivity analysis will identify key leverage points which have the most impact on model dynamics. These factors might be features of the environment or characteristics of the object.

OUTCOMES

- ❖ A model to predict the spatial and temporal changes in composition of a cellulose acetate object undergoing hydrolytic degradation.
- ❖ Sensitivity analysis to quantify how much different environmental or inherent factors impact the rate of degradation.

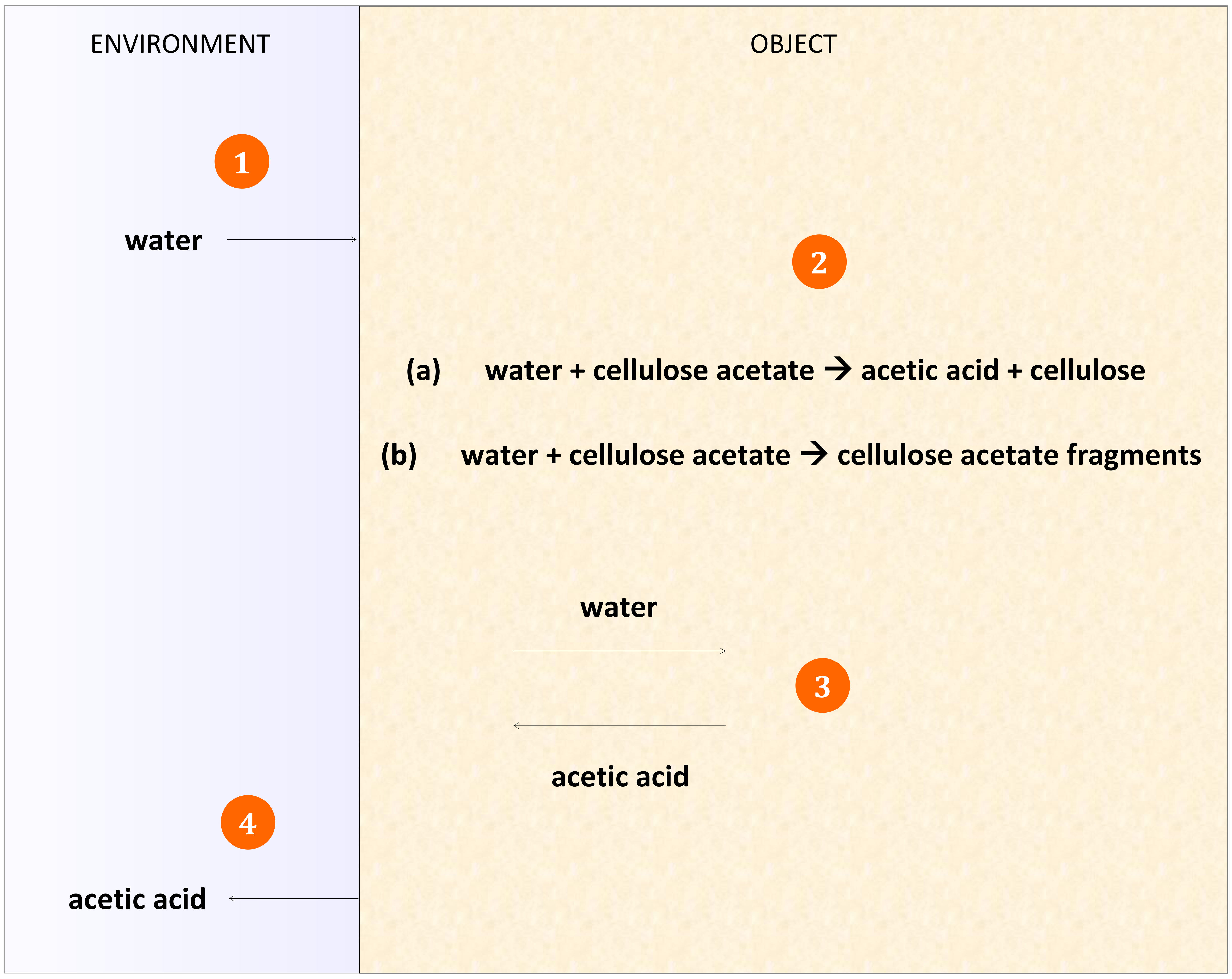

Fig. 1: A simplified process system model for hydrolysis in a cellulose acetate object. (1) Water vapour **absorbs** into the object from the environment; (2) hydrolysis **reactions** of cellulose acetate with water, (a) deacetylation and (b) glycoside bond cleavage; (3) water and acetic acid are transported through the object by **diffusion**; (4) acetic acid **evaporates** out of the object into the environment.

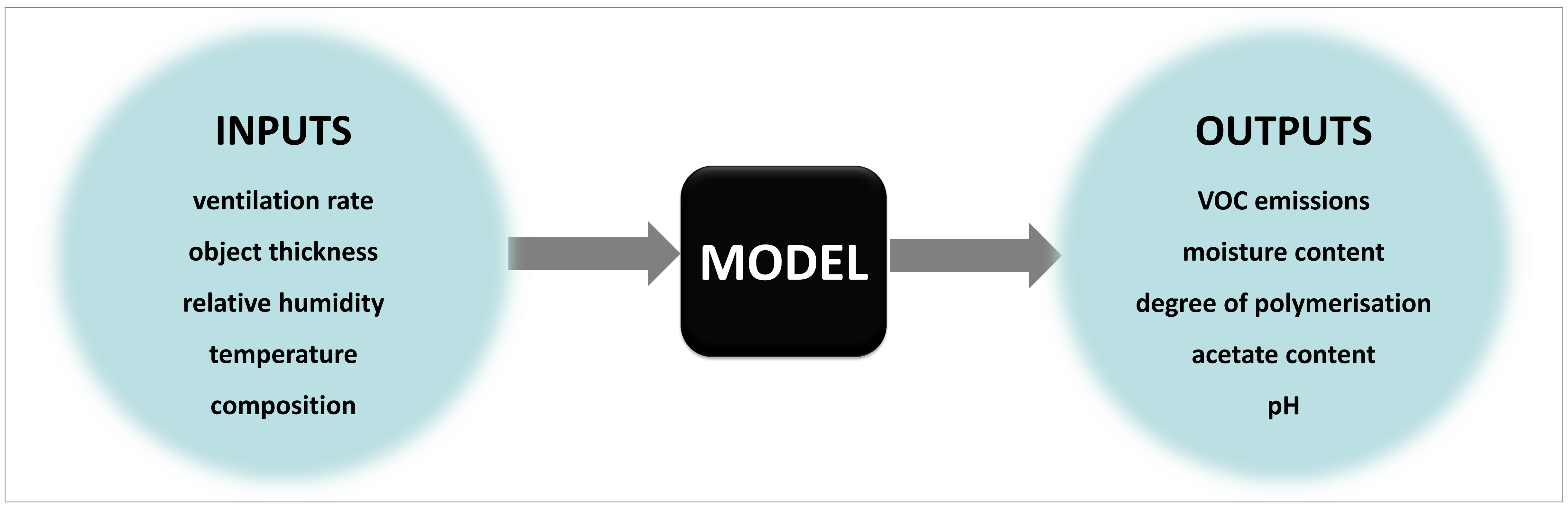

Fig. 2: Diagram showing how the model will convert inputs to outputs. The outputs are examples of the information that can be obtained by predictions of concentrations of chemical components.

BENEFITS & IMPACTS

A model is low-cost, non-destructive and may be more accurate for understanding degradation than experimental methods like accelerated ageing.

As a novel technique for studying the causes of material changes, the model could aid in research of the history of an artefact, e.g. to deduce details of its origins or use.

Conservation professionals will benefit from understanding how storage or display conditions affect degradation, and which characteristics make an object inherently unstable. The model can be used to support decisions in care of collections, e.g. risk mitigation or resource management.

The model will offer a new way for understanding degradation in modern polymeric materials. This knowledge can transfer horizontally to diverse applications from food packaging to medical devices.

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