Testing scientific theories using conceptual models: enzymatic degradation as a case-in-point example

The literature review, which fundamental to natural science, is getting more and more difficult for domain specialists due to the inexorable inflation of scientific papers. To facilitate the capture and computation of scientific domain knowledge, we proposed a method for assessing and integrating published scientific models. The method has been applied to understanding the mechanism limiting the enzymatic hydrolysis of cellulose, which is pivotal to research in a number of domains, including the production of biofuels.

► RESULTS

Our method consists of taking several concurrent scientific models and comparing them against a set of observations from other scientific publications. These observations describe target behaviours of the system that we want to first reproduce via simulation and then, ultimately, explain. These behaviours could for instance be the cellulose hydrolysis rate which first increases but then slows over the course of the reaction, or adding an enzyme mid-reaction to trigger an acceleration in the hydrolysis process. To reduce the context-dependent effect that reflects mainly into the quantitative measurements of experiments our method assumes the qualitative abstraction of the numerical values into a qualitative space and the mapping of scientific models into qualitative models. Simulations generated with the qualitative models are then compared against the target behaviours—if they prove coherent, then the model will convey a plausible scientific theory of that behaviour.

We applied our model to test assess two published kinetic models which are thought to explain the rate-limited hydrolysis of cellulose—one involving the processive saturation of enzyme-hydrolyzable cellulose surface, and one involving the presence of obstacles at the cellulose substrate surface disrupting and 'stalling' the enzymes. We showed that neither of the two models can fully explain all the target behaviours, whereas a third model integrating the first two is able to explain all the target behaviours.

► FUTURE OUTLOOK

This research borrows techniques and tools from Artificial Intelligence to mine and model knowledge and aspects of scientific reasoning. Work on the method is moving forward into an effort to automate the procedure—and thus apply it, for instance, to screen qualitative models for target behaviours or to facilitate the extraction of salient data from a complex set of publications.

Participants

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Read more

Testing scientific models using Qualitative Reasoning: Application to cellulose hydrolysis

(2017) Scientific reports

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