Applications of biomathematics to rumen microbiology

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FA and CFA are the major contributors, and QA and SKA the minor contributors, of the BA excreted in ruminant urine. It appears also that protozoa differ from bacteria in their metabolism of hydroxycinnamic and hydroxyalicyclic acids.

Applications of biomathematics to rumen microbiology.

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The majority of mechanistic models appearing in the ruminant literature are based on systems of ordinary differential equations (ODEs). There is a mathematically standard way of representing such models called the rate:state formalism [1]. The system under investigation is defined at time t by q state variables which represent properties or attributes of the system, e.g. microbial mass, quantity of substrate. The model then comprises q first-order ODEs describing how the state variables change with time. The terms on the right-hand sides of these ODEs represent rates of component processes, e.g. microbial synthesis, substrate utilisation, and can be calculated from the values of the state variables and the parameters. There are three types of solution to these models. (i) The system under investigation is in steady state and solutions are obtained by setting the differentials to zero and manipulating to give an algebraic expression for each component process (Type I solution). (ii) The system is in non-steady state and the

ODEs can be integrated analytically to give an expression for each state variable (Type II). (iii) The system is in non-steady state but the ODEs have to be integrated numerically (Type III). In this paper, we illustrate two applications drawn from our own work of mechanistic modelling in rumen microbiology based on the rate:state formalism with Type I and III solutions.

As an example of a Type I solution, an indirect approach to quantification of the fibrolytic anaerobic fungi in the rumen is described [2]. A model of the life cycle of anaerobic fungi, based upon observations of the life histories and growth kinetics of these organisms *in vitro* and *in vivo*, was constructed and solved in the steady state to determine the population of particle-attached fungal thalli from the concentration of free-swimming zoospores in rumen liquid. The values obtained are consistent with ruminal observations and with observations on faecal populations of fungal cysts or spores. As an example of a Type III solution, a model that simulates the dynamics of the rumen microbial ecosystem, with emphasis on the protozoa, is described [3, 4]. The model is driven by continuous inputs of nutrients and consists of 19 state variables representing the N, carbohydrate, fatty acid and microbial pools in the rumen. Several protozoal characteristics, e.g. engulfment and storage of starch, selective ruminal retention, are represented. The effects of dietary variations on microbial N turnover and recycling related to protozoal activity were simulated with diets containing roughages, e.g. fresh grass, maize silage, and variable proportions of concentrate, e.g. molasses, maize grain. High turnover rates and recycling levels were obtained with either maize silage, molasses or maize grain.

The results help explain differences in the efficiency of microbial protein synthesis.

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Computer simulation of cell wall degradation using cellular automata

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The kinetics of cell wall degradation by rumen micro-organisms *in vivo* are complex, and difficult to model mathematically in a biologically meaningful way. Measurement of cell wall degradation in sacco provides an overall degradation curve showing the rate at which cell wall material is lost. Similarly, measurement of gas production by rumen micro-organisms in

cubated with plant material *in vitro* provides information about the rate of cell wall degradation indirectly. The shape of these degradation curves is determined by many factors including forage quality, and has been the subject of several exponential models of cell wall degradation. The degradation curve itself represents an overall measure of the underlying kinetics, and provides useful information about the degradation process as a whole. However, many different factors combine to determine the overall shape of the degradation curve and it is almost impossible to assess their relative contribution by fitting curves to simple exponential models.

An alternative approach is to simulate the degradation process using a computer model. In this case, the continuous functions used to represent the overall degradation process in the exponential model are replaced by discrete numerical functions for which no analytical solution exists. The advantage of this approach is that the process can be modelled in a biologically meaningful way. Cellular automata are useful to describe processes that have a spatial component. An automaton is simply a computational 'cell' or unit which is arranged in an array of similar units. The automata process data in discrete steps or iterations, and share data with neighbouring automata. Typically an automaton can exist in a number of different states and obeys rules controlling the transition from one state to another. In the case of our cell wall degradation model, each automaton represents a small cube of cell wall material (or the solution in which a larger cube of plant material is incubated) and the automata rules have been defined to simulate the diffusion of cell wall degrading enzymes and the loss of cell wall material. The 'cut surface'

The 'cut surface' curve (solid line) represents degradation where all the cell wall is accessible to enzymes and the 'within tissue' curve (dashed line) represents degradation where access is restricted by other tissue.