- *Compile the model.* SMART will prompt you to save your changes first. Then it will check the model, if you did not do so yourself. When no errors are found, the 'Compile' dialogue appears. Press OK (on older systems, a (black) Command or DOS window may appear – close it when it is ready). If SMART indicates that the compiler cannot be found, check the installation notes to set the compilation preferences correctly. [In a computer lab, please contact one of the assistants.]
- *Run a simulation with the changed model.* Now births and deaths of hares and lynxes can be inspected. Try to use the experiment saved in the preceding part of the exercises. Because the model has changed, SMART issues a warning (just click OK) and ignores any available experiment outputs.

Case Study 1. A Simulation Model of Rumen Digestion and Passage Kinetics (150 min)

Objective

The aim of this case study is to exercise the process of translating biological processes, such as degradation, passage and absorption of nutrients, into a set of mathematical equations. Furthermore, knowledge on passage and degradation characteristics of feedstuffs, as well as on the fate of fermentation end products, is integrated in this case study. The case study consists of two parts. The first part should be completed in about 90 min and the second part in another 60 min.

A non-steady-state model of digestion kinetics (90 min)

Description of the system to be modelled

The process of fermentation and digestion is dynamic. Therefore, nutrient availability and utilization will fluctuate with time. The feed entering the reticulorumen can be characterized by a soluble fraction (S), a potentially degradable fraction (D) and an undegradable fraction (U). The degraded feed particles are substrate for microbial growth, with a concomitant production of the short-chain fatty acids: acetic acid (HAc), propionic acid (HPr) and butyric acid (HBu). Follow the instructions below to develop this model step-by-step: (i) the passage and digestion of the different feed fractions will be modelled in a non-steady-state condition (monitoring the fate of a single meal); (ii) the model will then be refined by adding microbial growth, fatty acid production and their absorption through the rumen wall.

Step-wise instructions to build this model in SMART

Build a model simulating passage and degradation of the different feed fractions through the rumen. Before building the model, make a flow chart and identify the proper pools (state variables) and fluxes (auxiliary variables). Always check

the units: state variables are quantities; fluxes are quantities per time unit. The following assumptions are made:

- The feed consists of S, D and U fractions. A single meal of 20 kg dry matter (DM) of dried grass is administered to a dairy cow with an empty rumen. Assume the S, D and U fractions of grass DM, measured by *in sacco* procedures, to be 30, 50 and 20%, respectively.
- The passage rate of the U fraction through the rumen (passageU, g h^{-1}) is proportional to the quantity of U present in the rumen. Assume the fractional passage rate of feed particles (k_p) to be 3% h^{-1}. Please do not enter the k_p as a number in the equation, but define the k_p as a constant in the 'Constants & Parameters' tab in SMART (constant k_p = 3% h^{-1}) and use this constant in the equation defining the flux leaving the U pool.
- The S fraction is passing through the rumen compartment with the liquid phase (passageS, g h^{-1}). For the passage rate of liquid, assume a constant fractional passage rate (constant k_l = 10% h^{-1}). The passage rate of S is proportional to the quantity of S present in the rumen. Apart from that, S material is also being degraded (degradationS, g h^{-1}). The degradation rate is proportional to the quantity of S present in the rumen. Usually, it is assumed that this material is degraded before it has the chance of leaving the rumen. The fractional degradation rate is, therefore, high: constant, k_{dl} = 200% h^{-1}.
- Like the U fraction, the D fraction is flowing out of the rumen compartment with the feed particles (passageD, g h^{-1}). Passage rate is proportional to the quantity of D present in the rumen. Apart from that, D material is also being degraded (degradationD, g h^{-1}). The degradation rate is proportional to the quantity of D present in the rumen. Assume the fractional degradation rate of D (constant, k_d) to be 2% h^{-1}.
- In the simulation, the cumulative quantities of D and S being degraded can be determined as follows: introduce additional pools for these quantities (name them cumdegradedD and cumdegradedS, respectively). Each of these pools has only one input: the degraded material leaving D and degraded leaving S, respectively. Not including any outputs from these pools assures a steady increase in pool size, collecting all degraded material, as the simulation progresses.

After building this model in SMART, compile the model and run it for a simulation time of 96 h (integration algorithm RKfixed, integration step 0.1 h) to answer the questions below. Create separate experiments for each question and save the simulation results with them.

Questions

1. Check the development of S, D and U with time. Does it match your expectations? How much of S, D and U is still in the rumen after 20 h? Record your answer in Table 25.1.

2. Now use straw instead of dried grass and answer question 1. Assume S, D and U to account for 10, 50 and 40% of the dry matter of straw and assume the

Table 25.1. Pool sizes of soluble (S), potentially degradable (D) and undegradable (U) material in the rumen, 20 h after a single meal.

Pool size at 20 h	Dried grass	Straw
S		
D		
U		

fractional degradation rate of D (k_d) to be 0.5 % h^{-1}. Compare and discuss the results.

3. Start a new experiment again. Now double the fractional passage rate of particles (k_p). How does this affect the degradation and passage rates at t = 20 h? Can you explain the difference? Would it be beneficial to the cow to double the fractional passage rate?

4. Look at the cumulative quantity of D and S being degraded in the rumen compartment during 96 h. What proportion of the ingested quantity of degradable (D) and soluble (S) material is actually degraded in the rumen after 96 h?

Microbial growth and short-chain fatty acids (60 min)

Description of the system to be modelled

In the first part of this case study, material degraded in the rumen has not been utilized for any purpose. In the cow, rumen degraded material is being used by microorganisms, which use it as fuel and building blocks. As a result, microbial biomass is produced. Furthermore, the microorganisms convert a substantial part of degradable material into short-chain fatty acids (i.e. acetic acid, Hac; propionic acid, Hpr; butyric acid, Hbu), which can be absorbed through the rumen wall and be used both as fuel and as a precursor for milk components by the cow.

Step-wise instructions to build this model in SMART

Extend the model you developed in the first part of this case study by a representation of rumen microbial biomass and the produced HAc, HPr and HBu. First, save the model under a new name. Again, identify pools and flows before actually entering the formulas into SMART. Where appropriate, introduce constants or parameters in the SMART model. The following assumptions are made:

- At time = 0 h, the microbial biomass in the rumen is close to 0 g (set the initial value of this state variable to 0). The pool of microbial biomass increases due to microbial growth, which occurs because microorganisms use degraded material in the rumen for their own growth (growthMB, g h^{-1}). Assume that all degraded material is converted to microbial biomass with an efficiency of 15% (constant MBeff = 0.15). Microbial biomass flows out of the rumen with the feed particles (passageMB, g h^{-1}) and it is assumed that

the passage rate is proportional to the microbial biomass present in the rumen (constant k_p = 3% h^{-1}).

- Microorganisms produce short-chain fatty acids from material that is degraded in the rumen (productionHAc, productionHPr, productionHBu, all in g h^{-1}). The efficiency with which degraded material in the rumen is converted into short-chain fatty acids is 70% (constant SCFAeff = 0.70). Of the total amount of short-chain fatty acids, the proportions of HAc, HPr and HBu are 65, 20 and 15%, respectively (on a weight basis) (constants: propHAc, 0.65; propHPr, 0.20; propHBu, 0.15). Short-chain fatty acids are water-soluble and therefore leave the rumen with the liquid phase (passageHAc, passageHpr, passageHBu, all in g h^{-1}), or are absorbed (absorptionHAc, absorptionHPr, absorptionHbu, all in g h^{-1}). For absorption of HAc, HPr and HBu through the rumen wall, assume that it is proportional to the quantity of the respective fatty acid present in the rumen and assume the fractional absorption rates to be constant: $k_{a,Hac}$ = 20% h^{-1}, $k_{a,Hpr}$ = 30% h^{-1} and $k_{a,Hbu}$ = 40% h^{-1}, for HAc, HPr and HBu, respectively.
- Include additional state variables to keep track of the cumulative quantity of microbial biomass (cumMB), HAc (cumHac), HPr (cumHpr) and HBu (cumHbu) produced from the single meal.

After including these formulas in the SMART model, compile it and run it for a simulation period of 96 h to answer the questions below. Again, create a separate experiment for each question.

5. Check the change of microbial biomass and the quantity of HAc, HPr and HBu with time. Does it match your expectations? At what time do these variables reach peak values?

6. Can you explain why the peak value of microbial biomass is about 50% of that of HAc (both in g)? Is that what you expected, considering the threefold higher efficiency of conversion of degraded material into HAc compared with microbial biomass?

7. Now use straw instead of grass, adapting S, D, U and k_d as earlier (see question 2) and answer question 5 again. Compare and discuss the results.

8. Look at the total quantity of microbial biomass, HAc, HPr and HBu produced from the single meal of dried grass within 96 h. What proportion of the degraded material (see question 4) is actually converted into short-chain fatty acids and what proportion into microbial biomass?

Case Study 2. Simulating the Growing Pig: Post-absorptive Utilization of Amino Acids, Glucose and Fatty Acids (240 min)

Objective

The aim of this case study is to exercise the process of the partitioning of nutrients through intermediary metabolism into protein and fat retention (i.e. growth)