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CHAPTER 16

Lactation

The flow of information downward from whole animal models to tissue and cellular models in the form of constraints and regulation, and the upward flow of information and insight gained in tissue and cellular models to whole animal models serves to facilitate advancement of knowledge and understanding of complex animal systems and identification of areas requiring experimental analysis.

Smith (1970)

16.1 INTRODUCTION

It was noted earlier (Chapters 3 and 4) that Smith (1970) formulated a dynamic model of the metabolism of a lactating cow using the KINSYM modeling language. The model was based solely on mass action equations, was very large and unwieldy, and was unstable, thus it required excessive solution times. Nevertheless, the model was based on a comprehensive analysis of data available at that time (summarized in Chapter 3) and incorporated many relevant concepts regarding ruminant metabolism. Deficiencies in our knowledge of ruminant adipose tissue, mammary gland and liver metabolism were identified as a result of Smith's analysis. Experimentation inspired by this modeling study and the resultant development of detailed models of metabolism in these three tissues were discussed in Chapters 12–14. These models remain imperfect but are providing bases for the identification, design, and interpretation of critical experiments and formulation of less detailed representations of lactating cow metabolism. In this, we were implementing the hierarchical concept of model development, which holds that detailed models of function at one level of organization (e.g. tissue) should provide the bases for construction of models of higher level (e.g. organism) functions. Improvement of the lactating cow model has occurred in parallel with emphases on reducing complexity and computing requirements, improving stability and enhancing the conceptual bases underlying the model.

The basic strategy utilized by Smith (1970) in representing the metabolism of a nutrient in a given tissue is depicted in Fig. 16.1. In the (KINSYM) modeling language, the metabolism of each nutrient utilized by a tissue

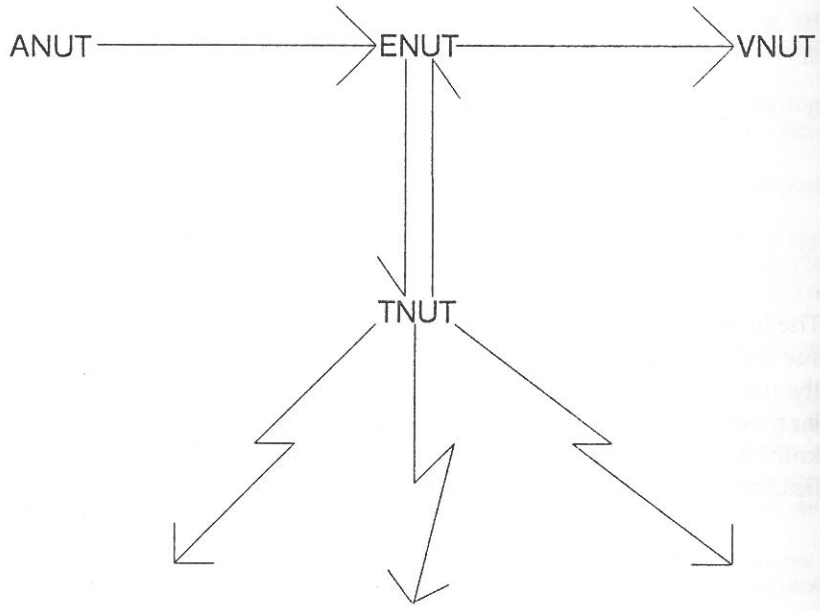

Figure 16.1 Smith model. Codes for abbreviations are arterial substrate concentration (ANUT), extracellular substrate concentration (ENUT), venous substrate concentration (VNUT) and tissue substrate concentration (TNUT).

required estimates of the arterial and venous, extracellular and intracellular pool sizes of each nutrient, blood flow rate to each tissue, and energy expenditure in each tissue. Several problems should be evident:

1. Blood flow estimates vary depending upon tissue energy requirements and this was not accommodated.
2. Tissue and extracellular concentrations of nutrients are variable and, largely, unknown.
3. Basic data available from arteriovenous (A–V) difference and radioisotope tracer experiments can uniquely define only two or three rather than the required five or six rate constants per nutrient.
4. Provisions for changes over time in rate constants specified for tissues could not be defined and, thus, were not included. Chronic effects of hormones, growth, environment, etc. upon tissue metabolic rates and patterns could not be simulated as would be appropriate throughout a lactation cycle.
5. The minimum number of differential equations required for each tissue were four times the number of nutrients used by that tissue (usually 3–4) plus equations associated with intermediary metabolism summing to a minimum of 15 differential equations per tissue. In addition to the problems with parameterization noted above, large numbers of equations led to high computation costs, even on today's computers. Turnover rates of intracellular metabolites are very high; up to 50–100 000 per day. In order to avoid unstable solutions, very short integration intervals were required ($5 * 10^{-5}$/day), with a corresponding increase in computation requirements.

This was clearly an overparameterized model constructed by experimental scientists with limited modeling experience. As a result of this experience, we identified research needs and gained essential insight into the modeling process. In essence this was a learning rather than a research experience, even though we intended the latter.

Several dynamic, mechanistic models of digestion and metabolism in lactating cows have been reported subsequently. These include the studies of Koong and Lucus (1973), Baldwin *et al.* (1987a–c) and Danfaer (1990). Of these, the model of Koong *et al.* (1982) incorporates the greatest number of empirical elements and the least number of representations of specific biochemical and physiological mechanisms. The model of Danfaer (1990) incorporates the greatest number of mechanistic equations and metabolic and physiological detail. All of these authors clearly stated that their models were research models, imperfect with regard to rigorous predictions of input:output relationships. Also, a great deal of additional modeling and experimental research would be required to adequately simulate the metabolism of lactating cows. On the other hand, evaluations of the several models have shown that dynamic, mechanistic models have several properties that improve their utility relative to static, factorial, empirical models. Most importantly, these models enhance our ability to anticipate effects of previous and current planes of nutrition upon current and future performance and have explanatory power that has helped advance our understanding of ruminant digestion and metabolism. We are not going to discuss the models of Koong *et al.* (1982) and Danfaer (1990) or other models in this chapter. Rather we will discuss a current version of a lactating cow model that evolved from the Smith (1970) model, through the Baldwin *et al.* (1987a–c) model and to the present. Our purposes are to illustrate how research models evolve as a combined experimental and modeling research program progresses. This could be considered a penultimate chapter in the sense that the model presented is the result of modeling and experimental contributions of the many workers and studies summarized in previous chapters of the book. On the other hand, penultimate is much too strong a word as this model does not represent a final integration of current knowledge of ruminant digestion and metabolism. It can and has been used to evaluate hypotheses and predict probable outcomes of possible interventions – genetic, pharmaceutical, nutritional. These evaluations certainly surpass in value the qualitative, intuitive evaluations of 'experts' available at the onset of model development and those available now, even though the

knowledge base available to 'experts' has advanced considerably. As stated by Forrester (1971),

> The objective of modeling is to combine the power of the human mind with the power of computers. Only the human mind can formulate a structure or a concept to which data can be fitted. However, the human mind is limited in its ability to analyze or anticipate the quantitative and dynamic behavior of the system described. The computer is ideal for the latter function. ...the computer can trace the behavior of the system through time in a rigorous fashion and thus provide correct – unbiased – implications of the assumptions, concepts, etc. that comprise the model.

In this context, the current model is certainly not penultimate. It represents a flawed attempt to fully utilize the combined powers of the human mind and computers in advancing our understanding of ruminants. It remains a research model in evolution and a transient stage in our continuing efforts to advance our understanding of ruminant digestion and metabolism and fully utilize this knowledge in the resolution of problems facing animal agriculture.

16.2 BACKGROUND ON MOLLY.CSL

Due to early constraints imposed by programming languages, e.g. the maximum of six-letter words in Fortran, most modelers employ acronyms or arbitrary names for entities within models. This habit is not restricted to computer specialists, however. Biochemists, physiologists, nutritionists, medical practitioners etc., also communicate in one or another form of mnemonics, shorthand or slang; perhaps this is a human trait that should not be blamed on programming languages. In models discussed in earlier chapters, many conventional abbreviations and mnemonics were used to identify state variables and metabolic transactions. In contrast, we have been fairly arbitrary, or perhaps just obscure, in naming our models. Well, not completely arbitrary – our model for the growth of male mice was named MICKEY; and our steer growth model was named SAM after a seemingly asexual character in a science fiction novel popular at that time. The first version of the current model of a lactating cow was named COW1 (Baldwin *et al.*, 1987a); how dull. When the digestion (Baldwin *et al.*, 1987c) and metabolism models were joined we named the result MYRTLE. My father once named a heifer calf Myrtle to honor a neighbor woman, but she was offended and my father had to change the calf's name. This woman did not like children and did not give out candy on Halloween, so one might say my name selection for the model was a bit of revenge. When a version of the model with inflated pool sizes (see below) was written to simulate full lactations, the model was named DAISY to indicate a 1-day integration interval. When diskettes with coding for MYRTLE and DAISY were transported home from the UK after my sabbatical, the MYRTLE diskette was scrambled. So as not to tempt fate further, DAISY became the parent version and remained so until early 1992. Over the 6 year period during which DAISY reigned, many piecemeal changes were introduced and the flow of biological logic became disjointed, e.g. DAISY got old; after all, most cows are culled before they complete six lactation cycles. Therefore, the program was reorganized, corrected and reformatted to form MOLLY, named for the very docile, patient cow to whom my father assigned the task of teaching me to milk by hand when I was 8 or 9 years old. Perhaps MOLLY will provide me and associates with a continuing opportunity to learn.

In contrast with the more or less mathematical format used to present models and equations in previous chapters, MOLLY will be presented in ACSL format in this chapter. Statements enclosed by quotes are comments ignored by ACSL, which we include during model development to record our reasoning, calculations, sources, etc. The comments in actual program MOLLY have been edited somewhat to delete slang, identify origins of numbers and add clarity. In ACSL format, each line of comment in a program must start and end with quote marks. When a comment is several lines long, the quote marks on each line are annoying. Therefore, we have eliminated the quote marks within comment blocks leaving only the initial (') and final (') quotes to identify comments. Commentary that was added to extend comments in the program *per se* is presented in italics.

16.2.1 Explanation of coding and identification of state variables

Most entities within the model are identified by a two-letter code, for example, Aa codes for amino acids. A notable exception is that the major body components are identified by single letters – B identifies body or carcass; V identifies viscera and its subcomponents including liver, udder, gastrointestinal tract, kidneys and heart; and F identifies adipose tissue. Transactions are identified as substrate code, product code and body site in which the reaction occurs, e.g. gluconeogenesis from amino acids in viscera (liver) is coded as AaGlV. Kinetic parameters for transactions are identified by prefixes and the transaction code, for example, KAaGlV identifies the affinity constant or K_s for amino acids and VAaGlV the metabolic capacity or V_{max} for gluconeogenesis from amino acids. Anabolic (AHOR) and catabolic (CHOR) hormones can act as modifiers of either V_{max} or K_s.

A number of additional prefixes and suffixes are used to identify terms associated with each state variable. These are listed as associated terms in the list of state variables below and include (using Aa as an example):

Aacor	correction factor used to expand pool size of Aa such that integration interval can be increased, for example, to 0.5 day for full lactation simulations (unitless; see Chapter 4)

CAa	concentration of Aa in plasma (mole/l)
DAa	differential equation for Aa (mole/day)
HCAa	heat of combustion of Aa (Mcal/mole) – when the factor F1 is set to 4.184 (default value in model) values are in MJ/mole. Sometimes HXx is used instead of HCXx
IAa	initial pool size of Aa (mole)
IAaF	factor used to compute IAa based upon body weight (mole/kg)
ICAa	initial concentration of Aa
IVAa	initial volume of distribution of Aa (l)
IVAaF	factor used to compute IVAa from body weight (l/kg)
VAa	volume of distribution of Aa (l)

STATE VARIABLES

Aa	plasma amino acids (mole); associated terms: Aacor, CAa, DAa, HCAa, ICAa, IAaF, IVAa, IVAaF, MWAa, VAa
abEav	absorbed energy average – a rolling average which influences activity of the $Na^+ K^+$-ATPase (Mcal, MJ); associated terms: IabEav, DabEav
Ac	plasma acetate (mole); associated terms: Accor, CAc, DAc, HCAc, IAc, IAcF, ICAc, IVAc, IVAcF, MWAc, VAc
Am	rumen ammonia (mole); associated terms: Amcor, CAm, IAm, IAmF, ICAm, MWAm
As	soluble ash (kg); associated terms: Ascor, CAs, DAs, IAs, IAsF, MWAs, FDAs
Ce	cellulose in small particle pool in rumen; associated terms: Cecor, DCe, HCCe, ICe, ICeF, MWCe
Cs	soluble carbohydrate pool in rumen (mole); associated terms: Cscor, CCs, DCs, ICs ICsF, MWCs, FDCs (FDOa, FDPe, FDCs)
Fa	plasma lipids, includes non-esterified fatty acids (NEFA) plus triacylglycerol (mole); associated terms: Facor, CFa, DFa, HCFa, IFa, IFaF, IVFA, IVFAF, MWFa, VFA
Fl	long-chain fatty acids in digestive tract (mole); associated terms: Flcor, CFl, DFl, HCFl, IFl, IFlF, MWFl
Gl	plasma glucose (mole); associated terms: Glcor, CGl, DGl, HCGl, IGl, IGlF, IVGl, IVGlF, MWGl, VGl
Ha	α-linked hexose polymers (starch) in rumen small particle pool (kg); associated terms: Hacor, DHa, HCST, IHa, IHaF, MWST
HaMi	microbes associated with starch in small particle pool (kg); associated terms: DHaMi, IHaMi, IHaMiF, HaMicr
Hb	β-linked hexose polymers (holocellulose) in rumen (kg); associated terms: Hbcor, DHb, IHb, IHbF

Hc	hemicellulose in rumen small particle pool; associated terms: Hccor, DHc, HCHc, IHc, IHcF, MWCe
HbMi	microbes associated with Hb (kg); associated terms: DHbMi, IHbMi, IHbMiF, HbMicr
LHOR	lactation hormones which enhance synthesis of udder enzymes (kg); associated terms: DLHOR, ILHOR, BST
Lp	large particles in rumen (kg); associated terms: Lpcor, DLp, ILp, ILpF
Mi	microbes in rumen (kg); associated terms: Micor, DMi, IMi, IMiF, HCMi, LpMi, SpMi, WAMi
MLKave	milk production rolling average over past two weeks (kg/day); associated terms: DMLKav, IMLKav
Ot	'other', insoluble ash plus lignin (kg); associated terms: Otcor, DOt, IOt, IOtF
Pb	protein in body (mole); associated terms: DPb, CPb, HCPx, MWPx, IPb, IPbF
Pi	insoluble protein in rumen (kg); associated terms: Picor, DPi, IPi, IPiF, HCPx, MWPx
PUN	plasma urea (mole); associated terms: PUNcor, DPUN, CPUN, IPUN, IPUNF, IVPUN, IVPUNF, PUNVOL, MWUR, HUR
Pv	protein in viscera (mole); associated terms: DPv, CPv, HCPx, MWPx, IPv, IPvF
RAa	rumen amino acids (mole); associated terms: RAacor, DRAa, IRAa, IRAaF, MWRAa
RAc	rumen acetate (mole); associated terms: RAccor, DRAc, IRAc, IRAcF, MWAc, HAc
RBu	rumen butyrate (mole); associated terms: RBucor, DRBu, IRBu, IRBuF, MWBu, HBu
RLa	rumen lactate (mole); associated terms: ULacor, DRLa, IRLa, IRLaF, MWLa, HLa
RLv	rumen liquid volume (l); associated terms: RLvcor, DRLv, IRLv, IRLvF
RPr	rumen propionate (mole); associated terms: RPrcor, DRPr, IRPr, IRPrF, MWPr, HPr
TDMIN	total dry matter intake (kg); associated terms: DDMIN
TMLKLm	total lactose production (kg); associated terms: DMLKLm
TMLKPm	total milk protein production (kg); associated terms: DMLKPm
TMLKTm	total milk fat production (kg); associated terms: DMLKTm
TsF	triacylglycerol in adipose tissue (mole); associated terms: DTsF, CTs, ITsF, ITsFF, MWTsF, HCTg

UENZ	udder enzymes (arbitrary units); associated terms: DUENZ, IUENZ
ULm	udder lactose (kg); associated terms: DULm
UMave	milk in udder – rolling average (kg); associated terms: DUMave, IUMave
UPm	udder milk protein (kg); associated terms: DUPm
UTm	udder milk fat (kg); associated terms: DUTm
VAcTsF	V_{max} for fatty acid synthesis from acetate in adipose tissue (mole/day); associated terms: DVAcTsF, IVAcTs

16.3 THE PROGRAM MOLLY.CSL

'This is an aggregated version of the 550 kg cow described by Smith (1970) and Baldwin and Smith (1971a,b). This version was developed to simulate and analyze overall energy transactions, within day patterns of nutrient use, longer term day-to-day patterns of nutrient use throughout a lactation or growth cycle and as an aid in the design of energy balance experiments.'

'The body weight of the reference cow used to parameterize the model was 550 kg. Empty body weight (EBW) of the initial reference cow was 500 kg; lean body mass (wtB) was 350 kg and includes skin, brain, kidney, muscle, skeleton and minor tissues; adipose tissue (wtF) was 75 kg and comprised of triacylglyceride (Ts = 60 kg) and cytoplasmic elements (wtcytF = 15 kg). Visceral weight (wtV) was 75 kg and included blood, gut, liver, heart and udder. Note that wtB and wtF would be expected to decrease in early lactation, while wtV would increase. The default initial empty body weight (IEBW) has now been changed to 650 kg with corresponding (linear) changes in weights of B, V and F.'

'Nutrient inputs were calculated for a 50:50 forage/concentrate ration and are continuous in the reference (default) state. Milk production was set at 30 kg/day and energy balance to zero. Milk was 3.5, 4.8 and 3.3%, respectively, of fat (expressed as tripalmitin and equivalent to 3.7% of true milk fat), lactose and protein. Input:output comments prior to each subsection of the model refer to this specific feeding/production condition.'

'This version has provisions that accommodate:

1. Different feeding frequencies, e.g. one or more meals per day or continuous feeding;
2. A wide range of diets specified as input by users;
3. Alternative feeding strategies, including specification of amounts of feed offered and conditional changes in rations offered;
4. Provisions for abomasal infusion of casein and BST and T3.'

'The default for this version is set for mid-lactation within day simulations. For long-term simulations, run overlays to increase pool sizes and reset mammary parameters are required.'

16.3.1 Initial section

```
INITIAL $ 'section of model'
  'BASIC UNITS
  TIME IN DAYS
  POOL SIZES IN KG OR MOLES
  CONCENTRATIONS IN MOLES/KG or LITER
  MOLECULAR WEIGHTS IN KG/MOLE
  FLUXES IN KG OR MOLES PER DAY'
```

16.3.2 Physical constants

```
'MOLECULAR WEIGHTS(MW)in kg/mole
  Fl = mixed long-chain fatty acids inplant lipids, Am = ammonia, Wa = water, Ch =
  choline'

CONSTANT
  MWSc = 0.171,MWOa = 0.134,MWPe = 0.187,MWSt = 0.162,MWFDLi = 0.619,...
  MWFl = 0.284,MWGy = 0.092,MWHc = 0.132,MWCe = 0.162,MWPs = 0.115,...
  MWPi = 0.115,MWNn = 0.322,MWAc = 0.060,MWPr = 0.074,MWBu = 0.088,...
  MWVa = 0.102,MWCh = 0.121,MWCs = 0.180,MWRAa = 0.133,MWUr = 0.060,...
  MWAm = 0.017,MWLa = 0.090,MWAs = 0.084,MWFa = 0.256,MWFDFA = 0.885,...
  MWCH4 = 0.016,MWAm = 0.014

'HEATS OF COMBUSTION (H_)

When F1 is set at 1.0, energy values are in Mcal/mole; when set at 4.184, values are in
MJ/mole. The HC for palmitate is 2.38. Values for HCMi and HCLg are in Mcal/kg.'

CONSTANT F1 = 1.0          $ 'Default condition is Mcal/mole.'
HCH4 = 0.211 * F1          $ HCAc = 0.209 * F1   $ HCPr = 0.367 * F1 $ HCBu = 0.524 * F1
HCGl = 0.673 * F1          $ HCGy = 0.397 * F1   $ HCFl = 2.657 * F1
'HCFl is value for stearate' $ HCFa = 2.712 * F1
HCCs = 0.673 * F1          $ HCHc = 0.562 * F1   $ HCPs = 0.656 * F1
HCNn = 1.2 * F1            $ HCCh = 0.4 * F1     $ HCUr = 0.152 * F1
HCOa = 0.3365 * F1         $ HFDLi = 5.23 * F1   $ HCLa = 0.336 * F1
HCTg = 7.57 * F1           $ HCLm = 1.346 * F1   $ HCAa = 0.627 * F1
HCTp = 0.3365 * F1         $ HCMi = 5.35 * F1    $ HCLg = 8.3 * F1
```

16.3.3 Initial conditions

The initial conditions specified for the model were derived almost exclusively from the data summaries of Smith (1970) which were presented in Chapter 3 as an illustration of the third step in the modeling process – collection of numerical data required to parameterize the mathematical statements.'

'In this context, initial conditions include not only initial pool sizes, body weight, body component weights and metabolite distribution volumes, but also initial fluxes. In the first version of the current model, initial conditions were presented as constants, e.g. iGP = 4.5E – 2. This restricted application of the model to a specific empty body weight (500 kg). Since many of the initial conditions specified are a linear function of body weight over a reasonable range and others vary as a function of body weight raised to, approximately, the 0.75 power (MBW), definitions of initial

conditions were later scaled to body weight or MBW to allow simulations of animals varying in initial body weight. The scaling factors should not be considered to be generally applicable, however. At a body weight of 550 kg, a lactating cow could clearly be thinner or fatter than the average depicted for the reference cow. Growing heifers might simply be growing, be growing and pregnant, or be growing, pregnant and lactating. In all cases, they differ significantly in body composition from the mature, non-pregnant, lactating reference cow. These differences could be quite critical in short-term simulations, in which case the modeler must develop an 'overlay' that corrects the initial conditions to reflect reality. Examples of some appropriate overlays are presented below as comments in the model. In long-term simulations, the model is a bit more robust in the sense that the model can be self-correcting. In other words, after several weeks of simulation, pool sizes adjust. However, body condition (composition) adjustments either take longer or do not occur during a given simulation. When the modeler has data adequate to specify initial conditions more accurately than the default, this should be done.'

'Initial conditions were set to allow for changes in initial empty body weight. This was done by dividing original pool sizes by 500 kg (the initial empty body weight of the reference cow). Thus, the IGl pool that was 4.5E – 2 became (4.5E – 2/500.0); an initial glucose factor (IGlF) of 9.0E – 5. The initial nutrient factors can then be multiplied by initial body weight to estimate initial pool size for each nutrient. Initial volumes for blood metabolites were similarly defined and become dynamic variables dependent on EBW changes during solution.'

```
'FOR THE MID-LACTATION REFERENCE (DEFAULT) STATE'
```

'Note that the default has been changed from 550 kg to 650 kg BW in this version.'

```
CONSTANT IEBW = 600.0,MatBW = 650.0,IBW = 650.0,abE = 0.435
   BWF = IEBW
   IabEav = abE * (BWF * * 0.75) * f1
```

'The term abEav is used in the dynamic section to accommodate effects of energy intake on energy expenditures due to specific functions such as ion transport. The coefficient 0.435 represents absorbed energy at mid-lactation feed intakes and should be adjusted for lower rates of milk production and non-lactating animals.'

```
CONSTANT IGlf = 9.0E – 5,IFaf = 5.0E – 4,IAcf = 1.18E – 3,IAaf = 7.5E – 5
CONSTANT IVGlf = 3.0E – 2,IVFaf = 1.0,IVAcf = 0.654,IVAaf = 3.0E – 2
CONSTANT IPbf = 1.18,IPvf = 0.252,ITsFf = 0.158
CONSTANT IHaf = 1.7E – 3,IHbf = 3.28E – 3,IHCf = 1.5e-3,ICef = 1.5e-3
CONSTANT ILpf = 6.78E – 3,IPif = 0.852E – 3,IOtf = 1.98E – 3,ICsf = 0.50E – 3
CONSTANT IAsf = 1.52E – 3,IAmf = 1.6E – 3,IMIf = 2.77E – 3,IFlf = 0.98E – 3
CONSTANT IRAcf = 8.0E – 3,IRPrf = 3.5E – 3,IRBuf = 1.2E – 3,IRAaf = 0.18E – 3
CONSTANT IMiHaf = 0.364E – 3,IMiHbf = 0.524E – 3,IPUNf = 7.0E – 3,IVPUNf = 1.0
CONSTANT IRLaf = 2.0E – 9,IRLvf = 0.1465, IBDNAf = 1.5e-4, IVDNAf = 1.5e-4
```

'IBDNAf and IVDNAf were set at 1.5E – 4 kg based upon rough estimates of maxima for lactating cows as no direct measurements were available. When data become available these initial values should be corrected. At

these values, the maximum EBW that the reference cow could achieve is 750 kg, but this is not likely under normal feeding conditions.'

'For initiation of full lactation simulations, initial rumen pools must be adjusted to lower intakes characteristic of late pregnancy. Example values for an intake of 7.0 kg * day^{-1} follow:

```
CONSTANT IHaF = 0.724E – 3,ILpF = 2.77E – 3,IHbF = 1.48E – 3,IPiF = 0.484E – 3
CONSTANT IOtF = 0.8E – 3,ICsF = 0.11E – 3,IAsF = 1.0E – 3,IAmF = 1.08E – 3
CONSTANT IMiF = 1.04E – 3,IFlF = 0.38E – 3,IRAcF = 3.89E – 3,IRPrF = 1.66E – 3
CONSTANT IRBuF = 0.58E – 3,IRAaF = 0.6E – 3,IMiHaF = 0.12E – 3,IMiHb = 0.19E – 3
CONSTANT IRLaF = 1.0E – 8,IRLvF = 1.4E – 4'
```

```
'CORRECTION FACTORS'
```

'As was discussed in Chapter 4, provisions for inflating pool sizes were introduced into the model to increase the maximum integration interval (MAXT) allowed during solution and, thus, increase solution speeds. For (default) within-day simulation control statements incorporate modest correction factors for the pool sizes of Cs, RAa, Am, Aa and Gl. These are coded _cor, as in Glcor. They are modest in the sense that a MAXT of 0.002 days is used and the pools continue to turn over every 8–10 min and approach a new steady state within 30–40 min. Since experimental measurements at intervals of less than one hour are unusual, these correction factors do not pose a problem in comparing simulated and experimental results, even when the perturbation of the system simulated is fairly dramatic.'

'When the overlay for long-term simulations is used to enable an integration interval of 0.5–1.0 day, some corrections are quite large, and up to two or three simulated weeks can be required to achieve a new steady state if large changes in feed intake or diet are simulated. When a large perturbation of the system is to be simulated, it is suggested that the short-term MAXT and correction factors be used to quickly approach the new steady state, and then the long-term MAXT and correction factors can be invoked to speed the solution. In order to allow this type of switch during a run, new correction factors must be specified during the run to override those defined in this initial section.'

```
CONSTANT Cscor = 10.0,RAacor = 10.0,Amcor = 10.0,Hacor = 1.0,RLvcor = 1.0
CONSTANT Hbcor = 1.0,RAccor = 1.0,RPrcor = 1.0,RBucor = 1.0,RLacor = 1.0
CONSTANT Micor = 1.0,Picor = 1.0,Lpcor = 1.0,Otcor = 1.0,Ascor = 1.0
CONSTANT Flcor = 1.0,MiHacr = 1.0,MiHbcr = 1.0
CONSTANT Facor = 1.0,Accor = 1.0,Aacor = 10.0,Glcor = 10.0,PUNcor = 1.0
CONSTANT Hccor = 1.0,Cecor = 1.0
'Computation of initial conditions'
   IGl = IGlf * BWF * Glcor          $ IVGl = IVGlf * BWF * Glcor
   IFa = IFaf * BWF * Facor          $ IVFa = IVFaf * BWF * Facor
   IAc = IAcf * BWF * Accor          $ IVAc = IVAcf * BWF * Accor
   IAa = IAaf * BWF * Aacor          $ IVAa = IVAaf * BWF * Aacor
   IPUN = IPUNf * BWF * PUNcor       $ IVPUN = IVPUNf * BWF * PUNcor
   IHa = IHaf * BWF * Hacor          $ ILp = ILpf * BWF * Lpcor
   IHc = IHcf * BWF * Hccor          $ ICe = ICef * BWF * Cecor
   IHb = IHbf * BWF * Hbcor          $ IPi = IPif * BWF * Picor
   IOt = IOtf * BWF * Otcor          $ IRLa = IRLaf * BWF * RLacor
```

```
ICs = ICsf * BWF * Cscor          $ IAs = IAsf * BWF * Ascor
IAm = IAmf * BWF * Amcor          $ IMi = IMif * BWF * Micor
IFl = IFlf * BWF * Flcor          $ IRLv = IRLvf * BWF * RLvcor
IRAc = IRAcf * BWF * RAccor       $ IRPr = IRPrf * BWF * RPrcor
IRBu = IRBuf * BWF * RPrcor       $ IRAa = IRAaf * BWF * RAacor
IMiHa = IMiHaf * BWF * MiHaCR     $ IMiHb = IMiHbf * BWF * MiHbCR
IBDNA = IBDNAf * BWF              $ IVDNA = IVDNAf * BWF
IPb = IPbf * BWF                  $ IPv = IPvf * BWF
ITsF = ITsFf * BWF
```

'The equations and parameter values for computing mammary metabolic capacity were adopted from Neal and Thornley (1983). Definition of terms:

```
LHOR = lactation hormone complex in kg
KLhor = degradation rate constant for Lhor
VUsyn = enzyme synthetic capacity per cell
Ucells = (arbitrary)number of secretory cells defines genetic potential of udder to pro-
duce milk
KUsyn = M–M type constant for hormone response
KUdeg = degradation rate constant for Uenz
KUdegM = degradation rate constant defining effect of udder milk (UMilk) on Uenz
Mave = average milk in gland over last 21 days (TaveM = 1/21)
KMdeg = half response point for degradation due to udder milk
THETA5 = defines slope of response
KMinh = factor defining inhibition of milk synthesis by milk
Mlkmax = maximum mammary capacity for milk'
CONSTANT KLhor = 0.0102,VUsyn = 1.0,KUsyn = 0.2
CONSTANT KUdeg = 0.1,KUdegM = 0.2,KMdeg = 27.0
CONSTANT THETA5 = 10.0,TaveM = 0.048,UMLKcr = 1.0
```

'Default udder parameters for mid-lactation reference state'

```
CONSTANT ILHOR = 0.395,IUENZ = 6860.0,IUMavf = 10.3,IUTmf = 0.36
CONSTANT IULmf = 0.494,IUPmf = 0.34,TavMLK = 0.143,Ucells = 1000.
```

'Parameters for initiation of lactation'

```
'CONSTANT ILHOR = 1.0,IUENZ = 520.0,IUMavf = 1.0,IUTmf = 0.01
CONSTANT IULmf = 0.1,IUPmf = 0.01,IMLKav = 10.0,TavMLK = 0.143'
```

'Administration of exogenous hormones expressed in multiples of endogenous concentrations'

```
CONSTANT BST = 1.0,T3 = 1.0
'UDDER PARAMETERS'
    MLKmax = 30.0 * UMLKcr  $ KMLKI = 3.0 * UMLKcr    $ IUMave = iUMavf * UMLKcr
    IUTm = IUTmf * UMLKcr   $ IUPm = IUPmf * UMLKcr   $ IULm = iULmf * UMLKcr
END $ 'OF INITIAL SECTION'
```


16.3.4 Dynamic, derivative section: digestive elements

```
DYNAMIC
    DERIVATIVE
    ALGORITHM IALG = 5      $'Fourth Order Runge Kutta; see Chapter 4 for alternatives.'
    NSTEPS NSTP = 1
    CONSTANT CINT = 7.0     $'Communication interval' MAXTERVAL MAXT = 0.002
                            $'Maximum integration interval'
    CONSTANT TSTP = 13.99   $'Time to stop simulation'
    TERMT ((T.GE.TSTP).OR.(STFLAG.EQ.1.0))
    TIME = T
```

'The following section is a PROCEDURAL that initiates values for non-state variables and transfers new values that are calculated algebraically from one integration step to the next.'

```
CONSTANT IOxup = 180.4,IFCM4Z = 44.08,IME = 2.7,IDMILK = 20.0
CONSTANT IpPm = 0.033,IpTm = 0.033,IMLKav = 28.0,IAtAdh = 0.0195
CONSTANT IcFa = 0.5E – 3,IcAc = 1.8E – 3,IcGl = 3.0E – 3,ITCH4 = 1.0E – 9
CONSTANT IDEI = 70.0, IMEI = 60.0
PROCEDURAL (FCM4Z,Oxup1,UMave,rtPOx,VGl,VAc,VFA,VAa,PUNvol,ME,...
    pTm,MLKave,AtAdht,EBW = T,IEBW)
    IF( T.LE.1.0E – 6) GO TO P
    rtPOx = rtPO            $ pTm = pTm1          $ FCM4Z = FCM4Z1
    AtAdht = atadh1         $ ME = ME1            $ Oxup1 = DOx
    UMave = UMave1          $ EBW = EBW1          $ BW = BW1
    VGl = IVGlf * EBW * Glcor $ VFA = IVFAf * EBW * Facor
    VAc = IVAcf * EBW * Accor $ VAa = IVAaf * EBW * Aacor
    PUNvol = IVPUNf * EBW
    go to Q
    P.. rtPOx = 5.3627
    Oxup1 = IOxup           $ UMave = IUMave      $ VGl = IVGl
    VAc = IVAc              $ VFA = IVFA          $ VAa = IVAa
    PUNvol = IVPUN          $ FCM4Z = IFCM4Z      $ ME = IME
    RLv = IRLv              $ EBW = IEBW          $ BW = IBW
    DMILK = IDMILK          $ MLKave = IMLKav     $ pPm = IpPm
    pTm = IpTm              $ AtAdht = IAtAdh
    Q.. continue
    END                     $ 'OF PROCEDURAL'
```

'A block diagram of the ruminant digestive element of the model with mnemonics and reference fluxes for each transaction is presented in Fig. 16.2. Figure 16.3 represents metabolic elements of the animal portion of the model. These are outputs from simulation runs that are generated by an output subroutine of the model program, which is available upon request. We use these outputs primarily as a diagnostic aid.'

(a) Feed composition and physical properties

'Essential inputs to the digestive element of the model are listed throughout the model (see Chapter 6 also). Obviously, the requirement that a diet be described in this detail imposes a severe limitation upon practical application of the model, since detailed data on diet composition are very few. Basic reasons for requiring such

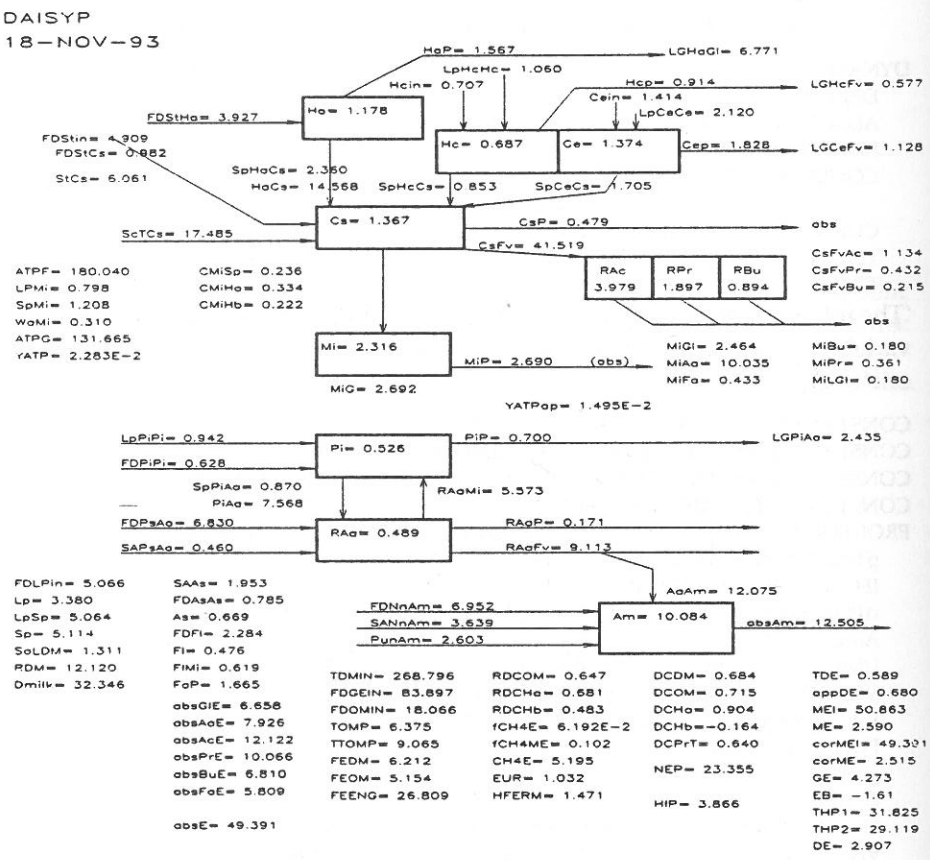

Figure 16.2 Diagrammatic representation of digestive element of the lactating cow model. Entities enclosed by boxes represent state variables and arrows indicate fluxes. Codes for abbreviations are defined in text and Baldwin *et al.* (1987b).

detail were 2-fold. The first was due to the fact that a primary reason why products of fermentation vary among diets is that the several components of the feed – soluble carbohydrates, starch, hemicellulose, cellulose, etc. – are utilized by different microbes whose fermentation products inherently differ. This concept has been widely accepted for a number of years and was amply demonstrated in the discussion of the Murphy et al. *(1982a) model discussed in Chapter 8. The results of Murphy* et al. *(1982a) were used to define the stoichiometric coefficients used in this model.'*

'The second reason underlying the detailed description of diet required as input to the digestive element is the requirement that input:output relationships in the model obey the first law of thermodynamics. Otherwise, the model could clearly not be used to investigate energetic relationships. This is easily achieved in the empirical, static, factorial models discussed in previous chapters because measurements underlying the systems are calculated by difference, as in the following:'

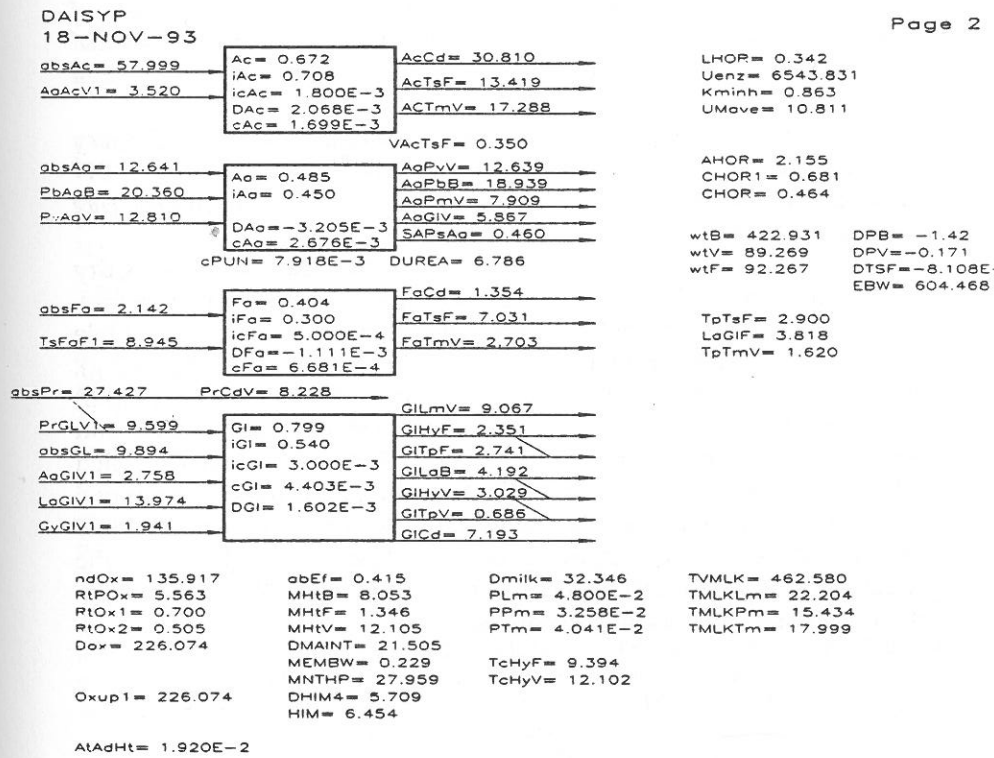

Figure 16.3 Diagrammatic representation of the metabolism model. Boxes indicate state variables. Arrows indicate fluxes.

'In comparative slaughter experiments such as,

$$HP = IE - FE - GE - UE - RE$$

and in indirect calorimetric experiments such as,

$$RE = IE - FE - GE - UE - HP.'$$

'Mechanistic models, by definition, incorporate specific precursor:product relationships and, as a result, energy contents of specific precursors and specific products must be explicitly represented. Murphy et al. *(1982a) determined that the proportions of products of fermentation from soluble carbohydrates, organic acids and pectins did not differ. However, the heats of combustion of these feed components differ significantly. Thus, they clearly cannot be treated in aggregate across feedstuffs. Similar considerations apply to plant lipids (Li) as opposed to yellow grease*

(Fat), to hemicellulose (Hc), to cellulose (Ce), and to organic acids (Ac, Bu, La) in silage.'

'Definition of physical characteristics of feed components, including estimates of starch solubility or availability to microbes and the particle size factor, are essential to accommodation of physical and temporal availabilities of nutrients to the rumen microbes.'

'The reference diet is 50% concentrate:50% chopped alfalfa hay fed at 15 kg/day on a continuous basis (0.625 kg/h). This is equivalent to an intake of 3% of BW (calculated at a EBW of 500 kg). This intake is almost adequate to keep the reference cow in energy balance.'

'The prefix fD indicates the fraction in feed of each nutrient in kg/kg dry matter. Codes are soluble carbohydrate (Sc), organic acids (Oa), pectins (Pe), lactate (La), lipid (Li), starch (St), hemicellulose (Hc), cellulose (Ce), soluble protein (Ps), insoluble protein (Pi), non-protein nitrogen (Nn), lignin (Lg), soluble ash (As), insoluble ash (Ai), volatile fatty acids as in silage (Ac,Bu) and organic matter (OM). Stsol is the fraction of starch that is soluble and must be input, since it is a physical characteristic of feed. For steam-rolled and ground cereal grains, this seems to be an adequate index of temporal availability of starch. For whole grains, milo and corn in particular, this is not adequate and rumen digestion coefficients are too high. PSF is the proportion of feed that enters the small particle pool directly and is a property of feeds and processing procedures.'

```
CONSTANT    fDSc = 0.06,fDOa = 0.05,fDPe = 0.06,fDLa = 0.0,fDLi = 0.04,...
            fDSt = 0.25,fDHc = 0.09,fDCe = 0.18,fDPs = 0.04,fDPi = 0.08,...
            fDNn = 0.03,fDLg = 0.04,fDAs = 0.04,fDAi = 0.04,fDAc = 0.0,...
            fDBu = 0.0,fDUr = 0.0,Stsol = 0.2,PSF = 0.4
            fDOM = 1.0 - fDAi - fDAs
CONSTANT    OBSME = 2.52,OBSDE = 3.00,OBSCH4 = 0.287
```

'In evaluations of the model, it is useful to input observed values, when available, so that these can be graphed versus model-predicted values in outputs from simulation runs. There are a number of observed values that can be defined as inputs to the model if desired. In this case, observed ME, DE and CH_4 values can be input. Model estimates of DE should always be below observed values, because microbial nucleic acids are all excreted in feces while, in reality, a significant portion of these are excreted in urine. Thus, simulated FE values are too high and UE values too low.'

'This procedural allows fat to be added from control language without recalculating proportions of other feed components. Thus, fDFAT is specified by setting FATADD to the proportion in the diet.'

```
CONSTANT FATADD = 0.0
PROCEDURAL (fDFAT = FATADD)
fDFAT = 0.0
IF (FATADD.GT.0.0) GO TO 2
GO TO 3

2.. factor = (1 - FATADD)
   fDFAT = FATADD          $ fDSc = factor * fDSc      $ fDOa = factor * fDOa
   fDPe = factor * fDPe    $ fDLa = factor * fDLa      $ fDLi = factor * fDLi
```



```
   fDSt = factor * fDSt    $ fDHc = factor * fDHc      $ fDCe = factor * fDCe
   fDPs = factor * fDPs    $ fDPi = factor * fDPi      $ fDNn = factor * fDNn
   fDLg = factor * fDLg    $ fDAs = factor * fDAs      $ fDAi = factor * fDAi
   fDAc = factor * fDAc    $ fDBu = factor * fDBu      $ fDOM = 1.0 - fDAi - fDAs
            GO TO 3

3.. CONTINUE
   END                     $ 'OF PROCEDURAL'
CWC = fDHc + fDCe + fDLg
FDGE1 = fDLi * 8.45 + fDSt * 4.154 + fDHc * 4.26 + fDCe * 4.154 + fDNn * 5.7
FDGE2 = (fDPs + fDPi) * 5.7 + fDLg * 8.3 + fDAc * 3.48 + fDBu * 5.95
FDGE3 = FDSC * 3.94 + FDFAT * 9.63
FDGE = (fDOa * 2.51 + fDPe * 3.6 + fDLa * 3.73 + FDGE1 + FDGE2 + FDGE3) * F1

'LARGE PARTICLE FRACTION OF FEED AND COMPOSITION'
```

'For simplicity, the decision was made to represent the large particle fraction as an aggregate state variable comprised of Ce, Hc, Lg, etc. rather than consider large particle pools of each component as a separate state variable. Implicit assumptions are that large particles cannot pass from the rumen, that no hydrolysis and fermentation of large particle components can occur, and that the conversion of large particles to small particles be totally dependent upon rumination. For subsequent equations it is essential that the composition of large particles be calculated.'

```
fLp = (fDCe + fdHc + fDLg + fDAi + fDPi) * (1.0 - PSF) $ 'Proportion of Lp'
fLpHc = fDHc * (1.0 - PSF)/fLp $ 'proportion of hemicellulose'
fLpCe = fDCe * (1.0 - PSF)/fLp $ 'proportion of cellulose'
fLpPi = fDPi * (1.0 - PSF)/fLp $ 'proportion of insoluble protein'
fOt = fDLg + fDAi $ 'combines lignin and silicates as Ot'
fLpOt = fOt * (1.0 - PSF)/fLp $ 'proportion of Ot'
fLgOt = fDLg/fOt

'TOTAL SOLUBLE SUGAR EQUIVALENT IN FEED
   Combines Oa,Pe, lipid glycerol and Sc as one fraction'
```

'As noted above and in Chapter 8, Murphy et al. *(1982a) found that fermentation patterns of Oa, Pe, etc., were very similar. They must be specified separately as inputs to the model for energetic reasons, but for purposes of simulating their fermentation can be combined into a common (Sc) pool.'*

'The algebra presented below converts kilograms of nutrients metabolized via a common pool to a common molecular weight basis. They were calculated as follows: (171 g Sc/mole Sc) * (0.5 mole Sc/mole Oa) * (134 g Oa/mole Oa)$^{-1}$ = (85.5 g Sc/mole Oa) * (134 g Oa/mole Oa)$^{-1}$ = 0.638 g Sc/g Oa.'

```
CONSTANT OaScSC = 0.638,PeScSC = 0.914,LiScSC = 0.138,
CONSTANT LaScSC = 0.95,HcCeCE = 1.02,FdFaSC = 0.097
OaSc = fDOa * OaScSC
PeSc = fDPe * PeScSC
LiSc = fDLi * LiScSC
FATSC = FdFAT * FdFaSC
fDScT = fDSc + OaSc + PeSc + LiSc + FATSC
'fDtot is a check to assure that DM/kg equals 1.0'
fDtot = fdsc + fdoa + fdpe + fdla + fdli + fdfat + fdst + fdhc + fdce + fdlg + fdps...
 + fdpi + fdnn + fdur + fdas + fdai + fdac + fdbu
```

'This provision was added to enable simulation of experiments where protein was infused per abomasum.'

```
CONSTANT INFPRT = 0.0  $ 'INFPRT = ABOMASAL INFUSION OF CASEIN'
                       'EXPRESSED IN KG/DAY'
```

(b) Feeding management and strategies

'Alternatives available for specifying feed inputs are:

RFEED1 – Multiple meals per day at intakes specified by user; during continuous feeding RFEED1 = 0.0.

RFEED2 – A specified feeding rate; can input total intake as observed in an experiment or an estimate of feed intake required for maintenance to which increments for lactation, growth and/or pregnancy can be added. Specified as default model input at 9.0 kg/day.

RFEED3 – An allowance for feed dry matter intake per unit of milk. Default for model is FDMLK = 0.33.

RFEED4 – Equation developed based upon voluntary feed intakes of lactating cows in southeastern US (Brown *et al.*, 1977).

RFEED5 – Equation derived from NRC (1989) equations for ME requirements of lactating cows (RFD5.A) with restrictions on ME intake due to NDF content of the ration offered (RFD5.B) according to Mertens (1985). RFD5.B is invoked when it is less than RFD5.A.

RFEED6 – Feeds the animal as a function of metabolic body weight. Utility of this provision is limited to simulation experiments in which this feeding strategy was used.

RFEED7 – Maintenance requirements of pregnant heifers and cows expressed as a function of days pregnant.

RFEED8 – Requirements of pregnant cattle for fetal growth as a function of days pregnant.

RFEED9 – Maintenance requirement of growing heifers.

RFED10 – ME requirement for weight gain in heifers.'

'Computation of RFEED1'

'For multiple feedings per day you must specify FDTM,FDINT and FDRAT (default values are 0.0). Feeding time (FDTM) is the time spent eating in each feeding interval (FDINT). FDRAT is kg dry matter consumed in each FDINT. Hourly feeding yields a FDINT of(1/24)0.04167. Summary equations are not always valid when using this mode.'

```
CONSTANT FDTM = 0.0,FDINT = 0.0,FDRAT = 0.0
```



```
PROCEDURAL (RFEED1 = T,FDTM,FDINT,FDRAT)
    RFEED1 = 0.0
    IF(FDRAT.EQ.0.0) GO TO 9
    IF(AMOD(TIME,FDINT).LE.FDTM) GO TO 8
    GO TO 9

8.. RFEED1 = FDRAT/FDTM
    GO TO 9

9.. CONTINUE
    END                          $ 'OF PROCEDURAL'
```

'Computation of RFEED2 AND RFEED3'

Basal feeding rate – RFEED2 – and kilogram feed allowed per kilogram milk – FDMLK – must be specified. This alternative (RFEED2 + RFEED3) is the default for full lactation studies.'

'The provision (Tavmlk, MLKave) in the section below was added originally to smooth feeding allowances for milk production over a period of time as opposed to feeding based upon milk production on a given day; the former approach is normally used during experiments. It turns out that this provision inadvertently has the property of lagging increases in feed intake in early lactation while milk production is increasing rapidly. Also, the delayed feed intake response which occurs several weeks after initiation of BST treatment is accounted for by this provision. Since models of feed intake that accommodate mechanistic explanations (and we know of none) for lags in feed intake responses to rapid changes in milk production, this provision has some useful, though fortuitous, properties.'

```
CONSTANT TavMLK = 0.072,RFEED2 = 9.0,FDMLK = 0.33
    RFEED3 = MLKave * FDMLK
    DMLKav = TavMLK * (DMILK – MLKave)
    MLKave = INTEG(DMLKav,iMLKav)
    'Computation of RFEED 4 and 5'
    RFEED4 USES THE BROWN ET AL. (1977) EQUATION W/O THE SEASON EFFECT
    RFEED5 USES THE MERTENS (1985) EQUATIONS
    THESE ARE CONTROLLED BY SETTING RFD4F OR RFD5F = 0.0(OFF)
    OR = 1.0(ON).'
    CONSTANT RFD4F = 0.0,RFD5F = 0.0,SEAF = 0.61,LAMMAX = 0.4,KLAM = 85.0
    CN = 20.854 – 27.076 * ((FCM4Z/2.204)/(MatBW * * 0.75)) $'LOWER LIMIT' 'FOR FIBER'
    CFF = CN * 0.018001 – CN * * 2 * 0.000557 $'CRUDE FIBER FACTOR' DMIN = 2.7182 *
    * (SEAF – 0.000827 * T + 0.148073 * ALOG(T + 0.00001) + … 0.33922 * ALOG(DMILK) +
    0.09926 * DMILK * PTM + 0.0675 * MatBW/(100.0 + CFF)) RFEED4 = DMIN
    RFEED5 = AMIN1(RFD5A,RFD5B)
    RFD5A = LAMDA * MatBW/NDF
    LAMDA = (1.0 + LAMMAX/((1.0 + KLAM/T + 1.0E – 4)))/100.0
    NDF = fDHc + fDCe + fDLg
    'CODING OF NRC (1989) DAIRY CATTLE EQUATION'
    NELREQ = NELMNT + NELLAC + NELD + NELP
    NELMNT = 0.08 * BW * * 0.75
    NELLAC = NELLKG * DMILK
    NELLKG = 0.3512 + 0.0962 * PTM * 100.0
    NELD = 5.12 * DBW
    PROCEDURAL (DBW = DWTB,DWTV,DWTTsF)
```

```
    DBW = DWTB + DWTV + DWTTsF
    IF(DBW.LT.0.0) DBW = 0.0
    IF(DBW.GT.0.5) DBW = 0.5
    END                          $ 'OF PROCEDURAL'

CONSTANT PDAYS = 305
```

'The default specification of PDAYS at 305 means that the reference cow is not pregnant during default simulations of a lactation. If otherwise must specify.'

```
PROCEDURAL (NELP = T,BW,PDAYS)
    IF(T.LT.PDAYS) NELP = 0.0
    IF(T.GE.PDAYS) NELP = 0.024 * BW * * 0.75
    END                          $'OF PROCEDURAL'
MEREQ = NELREQ/0.645

RFD5B = MEREQ/obsME
'Computation of RFEED6 which feeds at 2.0% of body weight'
CONSTANT FEEDBW = 0.02,RFD6F = 0.0
'Computation of RFEED 7 and 8.'

ENERGY REQUIREMENTS FOR PREGNANCY (FETUS & GRAVID UTERUS)
according to Moe and Tyrell (1972) and Ferrell et al. (1976).'
CONSTANT RFD7F = 0.0,RFD8F = 0.0
CONSTANT dconc = 90      $ 'day (post partum) of conception'
dpreg = t - dconc        $ 'days pregnant'
PROCEDURAL (RFEED7,RFEED8 = T,DPREG,obsME,BW,NELMNT)
MTME = NELMNT/0.645
RFEED7 = MTME/obsME
RFEED8 = 1.0E - 8 $ 'sets FMEREQ prior to conception to 1.0E - 8'
IF (T.LE.DCONC) GO TO 71
'MOE and TYRRELL equation (1972)'
MTME = (BW * * 0.75) * (0.567 * exp(0.0174 * dpreg))/1000
RFEED7 = MTME/obsME
'FERRELL - gross energy in gravid uterus at efficiency of 0.14 gives ME requirement in
Kcal/day - (0.14/1000 = 0.14E - 3) converts to Mcal/day'
FMEREQ = (69.73 * exp((0.0323 - 2.75E - 5 * dpreg) * dpreg)) * ... (0.0323 - 2 * 2.75E - 5 *
dpreg)/0.14/1000.0
RFEED8 = FMEREQ/obsME
71..CONTINUE
    END                          $'OF PROCEDURAL'

'Computation of RFEED9 and RFED10'
Feeding strategy for heifers from NRC (1989) up to breeding age.'
CONSTANT MNT = 0.077,LWG = 0.27,RFD9F = 0.0,RFD10F = 0.0
PROCEDURAL (RFEED9,RFED10 = RFD9F,rfd10f,MNT,...
LWG,obsME,ME,pTm,MLKave,BW)
RFEED9 = 1.0E - 8 $ RFED10 = 1.0E - 8
IF ((RFD9F.eq.0.0).AND.(RFD10F.eq.0.0)) GO TO 73
RFEED9 = ((MNT * (BW * * 0.75)) + (MLKave * (10 * pTm + 0.35)))/...
((1.37 * ME) - (0.138 * (ME * * 2)) + (0.0105 * (ME * * 3)) - 1.12)
RFED10 = (0.0686 * (BW * * 0.75) * (LWG * * 1.119))/...
((1.42 * obsME) - (0.174 * (obsME * * 2)) + (0.0122 * (obsME * * 3)) - 1.65)
GO TO 73
73.. CONTINUE
    END                          $'OF PROCEDURAL'
```



```
RFEED = RFEED1 + RFEED2 + RFEED3 + RFEED4 * RFD4F + ...
RFEED5 * RFD5F + RFEED6 * RFD6F + RFEED7 * RFD7F + ...
RFEED8 * RFD8F + RFEED9 * RFD9F + RFED10 * RFD10F
FDDMIN = RFEED $ DMIN = FDDMIN
FDOMIN = FDDMIN * fDOM
TDMIN = INTEG(DDMIN,1.0E - 8)
'FEEDING STRATEGIES'
LOGICAL FLAGGG
```

'This section provides for conditional changes in diet or other inputs based upon preset criteria and current status of the system. This is achieved by setting STFLAG to 1.0, which stops the simulation. Then the user can change the diet or other inputs and then continue the simulation with the CONTIN command.

STRAT1	provides for diet changes after 98 and 210 days of lactation.
STRAT2	provides for a diet change after 140 days of lactation.
STRAT3	provides for a diet change when milk production drops below 29.5 kg/day.
STRAT4	provides for a diet change when milk production drops below 29.5 and EBW is greater than 560 kg.
STRAT5	provides for changes when milk production drops below 20.0 kg/day.'

```
PROCEDURAL (STFLAG = T,DMILK,EBW,FLAGGG)
CONSTANT STRAT1 = 0.0,STRAT2 = 0.0,STRAT3 = 0.0,STRAT4 = 0.0,...
STRAT5 = 0.0,STRAT6 = 0.0,STRAT7 = 0.0
CONSTANT FLAGGG = .FALSE.
    'If flag is set, skip testing for this iteration, just reset to zero.'
    IF (STFLAG .EQ. 1.0) GOTO 41
    IF(STRAT1.EQ.1.0 .AND. (T .EQ.98.0 .OR. T.EQ.210.0))STFLAG = 1.0
    IF(STRAT2.EQ.1.0 .AND.(T.EQ.140.0)) STFLAG = 1.0
    IF(STRAT3.EQ.1.0 .AND.(DMILK.LT.29.5) .AND. (T .GT.50.0) .and. .not. FLAGGG)
    GOTO 47
    IF(STRAT4.EQ.1.0 .AND. (DMILK.LT.29.5).AND.(EBW.GT.560.0) .AND. (T.GT.50.0) .and.
    .not. FLAGGG) GOTO 47
    IF(STRAT5.EQ.1.0 .AND.(DMILK.LT.20.0) .AND. (T .GT.50.0) and not FLAGGG) GOTO
    47 GOTO 45
    41..STFLAG = 0.0
    GOTO 45
    47.. STFLAG = 1.0
    FLAGGG = .TRUE.
    GOTO 45
    45..CONTINUE
    END                          $'OF PROCEDURAL'
```

(c) Stoichiometric coefficients for fermentation

'For fermentation, three sets of coefficients are included. One is for, largely, forage diets (FORSET). The second is for 50:50 forage:concentrate diets

(MIXSET). The third set is for, largely, concentrate diets (CONSET). FORSET and CONSET are from Murphy *et al.* (1982a). MIXSET is a composite of the other two, since these apply to less than 50% and more than 50%, respectfully. Valerate was separated to 1/2Bu + 1Pr to maintain carbon and hydrogen balance. Values are in moles of VFA produced per mole of hexose fermented. One mole of glucose gives 2 moles of Ac or Pr but only one mole of butyrate. Amino acid fermentation stoichiometry is also from Murphy *et al.* (1982a). Even though the solution was non-unique (Chapter 8), it maintains C, H and O balance. The high proportion of propionate formed reflects Pr + 1/2 Bu from BCFA. CH4 is very highly dependent upon the proportion of BCFA produced. Stoichiometric coefficients for protein are expressed as moles VFA produced per mole AA fermented with an average 5.08 carbons per amino acid. Stoichiometries:'

```
PROCEDURAL (ScAcAc, ScPrPr, ScBuBu = FORSET, MIXSET, CONSET)
CONSTANT FORSET = 0.0,MIXSET = 1.0,CONSET = 0.0
   IF(FORSET.EQ.1.0) GO TO 10
   IF(MIXSET.EQ.1.0) GO TO 11
   IF(CONSET.EQ.1.0) GO TO 12
'FORSET'
10..ScAcAc = 1.38 $ ScPrP   = 0.40 $ ScBuB   = 0.11 $ ScLaL   =1.0E – 8
   StAcAc = 1.20 $ StPrPr  = 0.34 $ StBuBu  = 0.23 $ StLaLa  = 1.0E – 8
   HcAcAc = 1.14 $ HcPrPr  = 0.40 $ HcBuBu  = 0.23
   CeAcAc = 1.32 $ CePrPr  = 0.20 $ CeBuBu  = 0.24
   GO TO 13
'MIXSET'
11..ScAcAc = 1.14 $ ScPrPr  = 0.43 $ ScBuBu  = 0.215 $ ScLaLa =1.0E – 8
   StAcAc = 1.00 $ StPrPr  = 0.52 $ StBuBu  = 0.24 $ StLaLa  =1.0E – 8
   HcAcAc = 1.13 $ HcPrPr  = 0.49 $ HcBuBu  = 0.19
   CeAcAc = 1.45 $ CePrPr  = 0.20 $ CeBuBu  = 0.17
   GO TO 13
'CONSET'
12..ScAcAc = 0.90 $ ScPrPr  = 0.46 $ ScBuBu  = 0.32 $ ScLaLa =1.0E – 8
   StAcAc = 0.80 $ StPrPr  = 0.70 $ StBuBu  = 0.25 $ StLaLa =1.0E – 8
   HcAcAc = 1.12 $ HcPrPr  = 0.58 $ HcBuBu  = 0.15
   CeAcAc = 1.58 $ CePrPr  = 0.20 $ CeBuBu  = 0.11
   GO TO 13
13.. AaFvAc = 0.60,AaFvPr = 0.60,AaFvBu = 0.25,LaAcAc = 0.88,LaPrPr = 0.12
CONTINUE
   END                          $ 'OF PROCEDURAL'
```

'ADJUSTMENT OF STOICHIOMETRIC COEFFICIENTS FOR RPH'

'Stoichiometric coefficients are affected by pH. This is probably the reason Murphy *et al.* (1982b) found a relationship between amount of concentration in a ration and the stoichiometric coefficients. Therefore, provisions were added by Argyle and Baldwin (1988) for the pH to affect these coefficients. Data to do this were barely adequate. For this reason, the equations that should probably be sigmoidal are linear. Similarly the switch to a 'pure' lactate fermentation (below) at pH 5.4 may not be correct, since it is probably a logarithmic increase starting at 5.5. The changes in stoichiometric coefficients produced by the pH corrections parallel those suggested by the equation to CONSET as proportions of concentrate in the ration increased as formulated by Murphy *et al.* (1982b).'


```
PROCEDURAL (ScAc,ScPr,ScBu,ScLa,StAc,StPr,StBu,StLa = RpH,ScAcAc,...
   ScPrPr,ScBuBu,ScLaLa,StAcAc,StPrPr,StBuBu,StLaLa)
   ScAc   = ScAcAc $ ScPr  =  ScPrPr $ ScBu   =  ScBuBu $ ScLa=ScLaLa
   StAc   = StAcAc $ StPr  =  StPrPr $ StBu   =  StBuBu $ StLa =StLaLa
   IF(RpH.GE.6.2) GO TO 24
   IF(RpH.LE.5.4) GO TO 23
   ScAc   = 0.70 + ((RpH – 5.4)/0.8) * (ScAcAc – 0.70)
   ScPr   = 0.50 + ((RpH – 5.4)/0.8) * (ScPrPr – 0.50)
   ScBu   = 0.40 + ((RpH – 5.4)/0.8) * (ScBuBu – 0.40)
   StAc   = 0.66 + ((RpH – 5.4)/0.8) * (StAcAc – 0.66)
   StPr   = 0.82 + ((RpH – 5.4)/0.8) * (StPrPr – 0.82)
   StBu   = 0.26 + ((RpH – 5.4)/0.8) * (StBuBu – 0.26)
GO TO 24
23..  ScAc = 0.0 $ ScPr = 0.0 $ ScBu=0.0
      StAc = 0.0 $ StPr = 0.0 $ StBu=0.0
      ScLa = 2.0 $ StLa = 2.0
24.. CONTINUE
   END                          $ 'OF PROCEDURAL'
```

(d) Rumination, salivation and water dynamics.

'RUM is the proportion of time spent ruminating per unit time. There are separate equations for twice-daily feeding and continuous or multiple feedings. Rumination is shut off during feeding when the animal is fed twice daily. In continuous feeding, the animal ruminates during feeding, because rumination is needed for large particles to be broken down into small particles. Since the default is continuous feeding, RUMEQ is set to zero and ruminating rate (RUMF = RUM) to 0.33. When discrete feeding periods are used (FDINT does not equal FDTM), one should implement the rumination equation of Murphy *et al.* (1982b) by setting RUMF = 0.0 and RUMEQ = 1.0. This also enables resting salivation and drinking for the water balance equations below.'

```
DAY = 1.0
CWCf = 1.0 * (0.174 + 0.5085 * CWC)
CONSTANT RUMEQ = 0.0,RUMF = 0.333
CONSTANT MEAN1 = 0.0,MEAN2 = 0.054,AMP1FT = 0.1251,AMP2FT = 0.190
PROCEDURAL (RUM,RUMcor,RESTSA,RESTWA = RUMEQ,CWCf,DAY,...
TIME, AMP2FT,RUMF,FDINT,FDDMIN)
   RUM = RUMF
   REST = 1.0 – RUMF          $ RUMcor = 1.0
   RSTcor = 1.0               $ NOFEED = 1.0
   RESTSA = 0.85 * (EBW * * 0.75) * REST
   RESTWA = 1.4 * FDDMIN * 0.75
   IF(RUMEQ.EQ.0.0) GO TO 84
   IF(FDINT.EQ.0.5) GO TO 83
```

```
    AMPONE = AMP1FT * cos(6.283 * AMOD(TIME,DAY) + 1.9109)
    RUM = (CWCf + MEAN1) – AMPONE
    REST = (1.0 – (CWCf + MEAN1)) + AMPONE
    RESTSA = 6.0 * (RFEED/FDINT) * REST * RSTcor
    GO TO 84
83.. IF(FDDMIN.GT.0.0) NOFEED = 0.0
    AMPTWO = AMP2FT * cos(6.283 * (2 * AMOD(TIME,FDINT)) + 5.1)
    RUM = ((CWCf + MEAN2) – AMPTWO) * NOFEED
    REST = ((1.0 – (CWCf + MEAN2)) + AMPTWO) * NOFEED
    RSTcor = FDINT/(FDINT – RUMF/2)
    RUMcor = FDINT/(FDINT – FDTM)
    RESTWA = 0.0
    RESTSA = 0.0
    GO TO 84
84.. CONTINUE
    END                                    $ 'OF PROCEDURAL'
```

'Salivation, drinking, water flow through the rumen wall; rumen soluble, particulate and total rumen dry matter (RDM) are all variables that influence rumen volume. Rumen volume can be calculated based upon RDM/0.11, which is the default, or based upon water dynamics and osmolality when the rumen liquid volume equation (RLVEQ) is set to 1.0. The empirical equation for OSWA is not generally applicable and should not be used for continuous feeding and unusual diets, e.g. high salt, $NaHCO_3$, and, thus should be closely monitored when RLVEQ is set to 1.0.

'SALIVATION'

At RLVEQ = 0.0, the equation RESTSA = 6.0 * (RFEED/FDINT) * REST * RSTcor from above leads to the secretion of 60 l/day. When the animal is not eating, RFEED/FDINT is zero and RESTSA = 0.0. While the animal is ruminating, saliva flow is 85 l/day when RUM = 0.33 and EBW = 500kg.'

```
RUMSA = 2.41 * (EBW * * 0.75) * RUM
EATSA = 3.2 * FDDMIN                       $ 'l/kg FDDMIN'
SAin = EATSA + RESTSA + RUMSA              $ 'Total saliva flow'
```

'DRINKING'

'Drinking functions are based on 4.7 l/kg DM, with 70% being consumed during eating and only 75% of water consumed enters the rumen.'

```
EATWA = 3.30 * FDDMIN * 0.75
RESTWA = 1.40 * (RFEED/FDINT) * 0.75 * RUMcor * NOFEED
DRNKWA = EATWA + RESTWA
```

'Rumen volume based upon rumen dry matter CRDM'

```
SOLDM = Cs * MWCs/Cscor + Am * MWAm/Amcor + RPr * MWPr/RPRcor + RBu *
MWBu…
/RBucor + RAa * MWRAa/RAacor + As/Ascor + Fl * MWFl/Flcor + …
 RAc * MWAc/RAccor + RLa * MWLa/RLacor
RDM = Lp/Lpcor + Sp + SOLDM + Mi/Micor RUMVOL = RDM/0.11
'WATER DYNAMICS'
CONSTANT RLVEQ = 0.0
CONSTANT OsMolF = 1.70 $ 'OSMOLALITY FACTOR'
```



```
PROCEDURAL (RLv,PRDM = RDM,RLvEQ,SAin,DRNKWA)
    IF (RLVEQ.EQ.1.0) GO TO 28
    RLv = RDM/(0.11 – RDM)
    WAin = SAin + DRNKWA
    WAout = RLv * KWAP/RLvcor
    Go to 30
28.. WAin = SAin + DRNKWA
    WAout = RLv * KWAP/RLvcor
```

'Rumen Fluid OsMolality. As (soluble ash) multiplied by a factor to give moles of ions. MWAs = 0.084 was picked from $NaHCO_3$'

```
    ROsMol = (Cs/Cscor + Fl/Flcor + Am/Amcor + RAc/RAccor + …
    RPr/RPrcor + RBu/RBucor + RLa/RLacor + RAa/RAacor * OsMolF…
     + (As/MWAs)/AScor * OsMolF)/RLv
    OsWA = 0.74 * ((ROsMol – 0.280) * 1000) – 41.0     $ 'From Dobson et al. (1970)'
    DRLv = WAin – WAout + OsWA
    RLv = INTEG(DRLv,IRLv)                             $ 'Rumen liquid volume'
    PrDM = RDM/(RDM + RLv)                             $ 'percent rumen dry matter'
    GO TO 30

30.. CONTINUE
    END                                    $ 'OF PROCEDURAL'

DLRATE = WAout/RLv
'RUMEN pH'
```

'Rumen pH influences stoichiometry of fermentation (above) and hydrolytic rate constants for cellulose and hemicellulose. This is most relevant when meal rather than continuous feeding is implemented. However, in the default it is left on (RpHCON = 1.0,FIXDpH = 0.0). When RpHCON = 0.0, fixed pH (FIXDpH = 6.8) must be specified.'

```
CONSTANT VFAeff = 0.015,RpHCON = 1.0,FIXDpH = 0.0
RpH = (7.20 – (VFAeff * cVFA + 0.0015 * (cRLa * 1000))) * RpHCON + FIXDpH
TVFA = RAc/RAccor + RPr/RPrcor + RBu/RPrcor
cVFA = TVFA/(RLv/RLvcor) * 1000 $ 'cVFA in mMoles/liter'
```

(e) Passage rate constants

```
CONSTANT KSPP = 1.33,KWAP = 3.5
KSPP = 2.67 * (FDDMIN/(EBW * * 0.75)) + 1.00
KWAP = 1/((0.028 * (EBW * * 0.75)/FDDMIN) + 0.16)
```

'KSPP and KWAP are fractional turnover rates/day. Equations derived by regression equations'

(f) Large and small particle pools (Lp and Sp in kg)

```
CONSTANT KLpSp = 4.50 $'Questions such as Should KLpSp be a function of the physical properties of feeds; should KLpSp be a function of fermentation rate; and, should entry be lagged for hydration are unresolved at present.'
DLp = FDLpin – LpSp
FDLpin = fLp * FDDMIN $ 'LARGE PARTICLES'
```

```
LpSp = KLpSp * Lp/Lpcor * RUM
Lp = INTEG(DLp,ILp)
  'SMALL PARTICLE POOL SIZE (in kg)'
Sp = Ha/Hacor + Hb/Hbcor + Pi/Picor + Ot/Otcor $ 'SMALL PARTICLES'
SpPer = Sp/(Sp + Lp)
```

'Provisions for association of microbes with small particle Ha(MiHa) and Hb (MiHb) were added to prevent increases in microbes from Ha fermentation from increasing the digestion of Hb (due to more microbes) and vice versa, i.e. to give specificity to microbes associated with small particles based on the substrate upon which they grew.'

'In the first version of the model, cellulose (Ce) and hemicellulose (Hc) were dealt with in aggregate as holocellulose (Hb). Later, it was recognized that this simplification led to some significant errors due to the fact that fermentation products from these two entities differ significantly, as can their relative rates of hydrolysis when a wide range of feedstuffs were considered. Therefore, the decision was made to treat Ce and Hc as separate state variables. In some sections of the model, including the following depiction of the association and release of microbes from small particles of fiber, this separation could have added considerable complexity. Therefore, the simple, original representation and consideration of Hb as a state variable dependent upon Ce and Hc hydrolysis was retained (see section on fiber digestion). Some subtle errors arise from the facts that the Ruminococci *hydrolyze Ce and Hc and ferment the products of hydrolysis, while* Fibrobacter succinogens *hydrolyzes both but only ferments the products of cellulose hydrolysis. In the absence of detailed models of the rumen ecology we must accept these subtle errors, which may well be small at this level of aggregation.'*

```
CONSTANT KMiHa = 1.56,KMiHb = 0.41,VMiHa = 0.85
CONSTANT VMiHb = 0.85,KMiHaF = 0.095,KMiHbF = 0.041
   Csin = ScTCs + StCs + HaCs + HcCs + CeCs          $ 'Fractions of Cs entry'
   fCsHa = HaCs/Csin                                 $ 'attributed to Ha and Hb'
   fCsHb = (HcCs + CeCs)/Csin                        $ 'hydrolysis.'
   HaMiP = (HaMi/MiHaCr) * KSPP
   HbMiP = (HbMi/MiHbCr) * KSPP                      $ 'Passage of microbes in'
   OtMiP = OtP * cMiSp                               $ 'association with Sp'
   PiMiP = PiP * cMiSp
   SpMiPi = OtMiP + PiMiP + HaMiP + HbMiP
   CsMiG = MiG * (CsFv * CsFvAT/ATPF)                $ 'Proportions of microbial'
   HaMiG = CsMiG * fCsHa                             $ 'growth attributable to'
   HbMiG = CsMiG * fCsHb                             $ 'Cs formed from Ha and Hb'
                                                     'hydrolysis.'
   cMiHa = (HaMi/MiHaCr)/(Ha/Hacor)                  $ 'Concentration (kg/kg) of'
   cMiHb = (HbMi/MiHbCr)/(Hb/Hbcor)                  $ 'microbes associated with'
                                                     'Ha and Hb.'
   SpMiHa = KMiHa * Ha/Hacor * cMiSp                 $ 'Microbes attached'
   SpMiHb = KMiHb * Hb/Hbcor * cMiSp
   HaMiR = cMiHa * SpHaCs                            $ 'Microbes already associated
                                                     with Sp potentially released
                                                     due to hydrolysis of particulate
                                                     substrates.'
   HbMiR = cMiHb * SpHcCs + cMiHb * SpCeCs
```



```
   HaMiF = VMiHa/(1.0 + KMiHaF/((Ha/Hacor)/Sp))      $ 'Fraction of potentially
                                                     released microbes actually
                                                     released.'
   HbMiF = VMiHb/(1.0 + KMiHbF/((Hb/Hbcor)/Sp))      $ 'Dependent on fractions of
                                                     Ha and Hb in Sp where
                                                     maximum retention on Sp
                                                     is 0.85 of those potentially
                                                     released.'
   MiHaMi = HaMiF * (HaMiG + HaMiR)                  $'Microbes on particles'
                                                     'and'
   MiHbMi = HbMiF * (HbMiG + HbMiR)                  $'those grown from Ha at Hb
                                                     hydrolysis and fermentation
                                                     which remain in association
                                                     with SP.'
   DHaMi = SpMiHa + MiHaMi – HaMiP – HaMiR
   DHbMi = SpMiHb + MiHbMi – HbMiP – HbMiR
   HaMi = INTEG(DHaMi,iMiHa)
   HbMi = INTEG(DHbMi,iMiHb)
   'Starch (St in kg) or α-hexose (Ha in kg) hydrolysis and passage'
CONSTANT KHaCs = 6.0
   DHa = FDStHa – HaP – SpHaCs
   FDStin = fDSt * FDDMIN
   FDStCs = FDStin * Stsol
   FDStHa = FDStin – FDStCs
   HaP = Ha/Hacor * KSPP
   SpHaCs = KHaCs * Ha/HAcor * cMiHa
```

'Note that all equations for the hydrolysis of components of small particles are mass action in nature. Units in these equations are KHaCs in day^{-1} times Ha in kilogram times cMiHa in kg/kg = kg/day. The premise is that once a microbe is associated with a particle, substrate concentration is saturating and, thus, the rate of hydrolysis is a function of hydrolytic capacity (kHaCs) per unit of microbes in association with the substrate. Also, the equation above for the association and release (HaMiR and HaMiF) from particulate substrates sets a maximum for associated microbes (MiHaMi) dependent upon the amount of substrate available. Thus, the equations are mass action in form but are highly constrained such that implicit maximal rates of hydrolysis are specified.'

```
   RDCHa = 1.0 – HaP/FDStin
   Ha = INTEG(DHa,IHa)
```

'Holocellulose (Hb = Hc + Ce; Hc + Ce in kg) hydrolysis and passage'

Rates of hemicellulose and cellulose hydrolysis vary with type of forage. The following procedural allows for adjustment of KHcCs1 and KCeCs1 to grasses, legumes and corn silages. The default setting is for legumes.'

```
CONSTANT Grass = 0.0,Legume = 1.0,CornSi = 0.0,GKCeCs = 9.0
CONSTANT GKHcCs = 7.0,LKCeCs = 6.0,LKHcCs = 6.0,CKCeCs = 9.0
CONSTANT CKHcCs = 9.0
PROCEDURAL (KCeCs1,KHcCs1 = Grass,Legume,CornSi,GKCeCs,...
GKHcCs,LKCeCs,LKHcCs,CKCeCs,CKHcCs)
   IF(Grass.EQ.1.0) GO TO 14
```

```
    IF(Legume.EQ.1.0)
GO TO 15 IF(CornSi.EQ.1.0) GO TO 16
    'Grass'
    14.. KCeCs1 = GKCeCs $ KHcCs1 = GKHcCs
    GO TO 17
'Legume'
    15.. KCeCs1 = LKCeCs $ KHcCs1 = LKHcCs
    GO TO 17
'CornSi'
16.. KCeCs1 = CKCeCs $ KHcCs1 = CKHcCs
    GO TO 17
17.. Continue
    END                          $ 'OF PROCEDURAL'
```

'The following equations were devised to accommodate RpH effects on fiber digestion. The equation should probably be sigmoidal from pH 7.0 to pH 5.5, with the steepest decrease between 6.2 and 5.5; but, there are not enough data to fit that form.'

```
PROCEDURAL (KHcCs, KCeCs = RPH, KHcCs1, KCeCs1)
    KHcCs = KHcCs1 $ KCeCs = KCeCs1
    IF(RpH.GE.6.2) GO TO 22
    KHcCs = KHcCs – (KHcCs * 1.875 * (6.2 – RpH))
    KHcCs = AMAX1(KHcCs,0.0)
    KCeCs = KCeCs – (KCeCs * 1.875 * (6.2 – RpH))
    KCeCs = AMAX1(KCeCs,0.0)
    GO TO 22
22.. CONTINUE
END $ 'OF PROCEDURAL'
```

'The effects of added dietary fat on organic matter digestibility depicted below were added 12/90 but are very tentative, as the linear slope was derived from ± fat data.'

```
CONSTANT KfatHb = 0.06
    DHc = Hcin + LpHcHc – SpHcCs – HcP
    RHcin = fDHc * FDDMIN
    Hcin = RHcin * PSF
    LpHcHc = LpSp * fLpHc
    SpHcCs = KHcCs * (1 – (FDFAT/fDLi * KFATHb)) * Hc/Hccor * cMiHb
    HcP = KSPP * Hc/Hccor
    RDCHc = 1.0 – HcP/RHcin
    Hc = INTEG(DHc,IHc)
    DCe = Cein + LpCeCe – SpCeCs – CeP
    RCein = fDCe * FDDMIN
    Cein = RCein * PSF
    LpCeCe = LpSp * fLpCe
    SpCeCs = KCeCs * (1 – (FDFAT/fDLi * KFATHb)) * Ce/Cecor * cMiHb
    CeP = KSPP * Ce/Cecor
    RDCCe = 1.0 – CeP/RCein
    Ce = INTEG(DCe,ICe)
    DHb = Hbin + LpHbHb – SpHbCs – HbP
    Hbin = Cein + Hcin
    LpHbHb = LPCece + LpHcHc
    SpHbCs = SpCeCs + SpHcCs
```



```
RDCHb = 1.0 – HbP/(FDDMIN * (fDHc + fDCe))
Hb = INTEG(DHB,IHb)
```

Insoluble protein (Pi in kg) hydrolysis and passage

```
CONSTANT KPiAa = 7.0, KFATPi = 0.03
```

'KPiAa is probably a variable across feedstuffs and would be a variable if there were data to formulate an appropriate equation. Tentative effects of added dietary fat on protein degradability were added in 12/90. This effect is poorly supported.'

```
    DPi = FDPiPi + LpPiPi – SpPiAa – PiP
    FDPiPi = fDPi * FDDMIN * PSF
    LpPiPi = LpSp * fLpPi
    SpPiAa = KPiAa * (1 – (FDFAT/fDLi * KFATPi)) * Pi/Picor * cMiSp
    PiP = KSPP * Pi/Picor
    TPRTin = (fDPs + fDPi + fDNn) * FDDMIN
    RDCPRT = (TPRTin – PiP – (RAaP * MWAa))/TPRTin
    Pi = INTEG(DPi,IPi)
```

Lignin and insoluble ash (Ot in kg) passage

```
    DOt = LpOt + fDOt - OtP
    LpOt = LpSp * fLpOt
    FDOt = FDDMIN * fOt * PSF
    OtP = KSPP * Ot/OTcor
    Ot = INTEG(DOt,IOt)
```

(g) Soluble pools

Soluble carbohydrates (Sc in kg; Cs in Moles)

```
CONSTANT VCsFv = 1000,KCsFv = 0.009
DCs = ScTCs + StCs + HaCs + HcCs + CeCs – CsFv – CsMi – CsP
cCs = (Cs/Cscor)/(RLv/RLvcor)
```

'These equations convert kg of carbohydrates to moles of hexose equivalents.'

```
    ScTCs = FDScT * FDDMIN/MWSc
    StCs = FDStCs/MWSt
    HaCs = SpHaCs/MWSt
    HcCs = SpHcCs/MWHc * 0.833
    CeCs = SpCeCs/MWCe
    CsFv = VCsFv * WaMi/(1.0 + KCsFv/cCs)
```

'Note that all equations associated with the fermentation and utilization of soluble nutrients are of the Michaelis–Menten type in form. In a number of cases, including soluble carbohydrates (Cs), amino acids and peptides (Aa), concentrations of the nutrients in rumen fluids are far below the apparent affinities of microbes for the nutrient and, thus, mass action equations would serve equally well under most conditions. Two observations led to adoption of the equation form used: there are and have been experiments run using diets and conditions where concentrations of soluble nutrients have been high enough to approach saturation (see Argyle and

Baldwin, 1989, for examples). Some of these have been adequate to parameterize non-linear equations. In general, equations depicting saturation kinetics are more stable and help to avoid aberrant solutions that are sometimes associated with the use of mass action kinetics.'

```
CsMi = MiG * (CsMiG1 * G1 + CsMiG2 * G2)
CsP = KWAP * Cs/Cscor Cs = INTEG(DCs,ICs)
```

Amino acid (RAa in moles) metabolism

```
CONSTANT VRAaFv = 407.0,cSaPs = 0.002,KRAaFv = 0.0064
DRAa = FDPsAa + PiAa + SaPsAa – RAaFv – RAaMi – RAaP
cRAa = (RAa/RAacor)/(RLv/RLvcor)
FDPsAa = fDPs * FDDMIN/MWPs
PiAa = SpPiAa/MWPs
RAaP = KWAP * RAa/RAacor
SaPsAa = cSAPs * SAin
RAaFv = VRAaFv * WaMi/(1.0 + KRAaFv/RAa)
RAaMi = MiG * AaMiG2 * G2
RAa = INTEG(DRAa,IRAa)
```

Ammonia (Am in moles) metabolism

```
CONSTANT NnAmAM = 3.8,AaFvAM = 1.325,KAmabs = 12.4, UrAmAm = 2.0
CONSTANT VPUNAm = 5.67E – 2,KPUNAm = 0.007,KIAm = 0.003
DAm = FDNnAm + AaAm + SaNnAm + PUNAm – absRAm – AmMi + FdUrAm
FDUrAm = fDUr * FDDMIN * UrAmAm/MWUr
cAm = (Am/Amcor)/(RLv/RLvcor)
cPUN = (PUN/PUNcor)/PUNvol
FDNnAm = fDNn * FDDMIN * NnAmAM/WNn
AaAm = RAaFv * AaFvAm
SaNnAm = cPUN * SAin * UrAmAm
PUNAm = (VPUNAm * (EBW * * 0.75)/(1.0 + KPUNAm/cPUN + cAm/KiAm)) *
        UrAmAm
'Pun transport across rumen wall inhibited by Am.'
absRAm = KAmabs * Am/Amcor
AmMi = MiG * (AmMiG1 * G1 + AmMiG2 * G2) Am = INTEG(DAm,iAm)
```

Soluble ash (As in kg)

```
CONSTANT fSaAs = 0.0085,KAsabs = 58.0
DAs = FDAsAs + SaAs – AsP – absRAs
FDAsAs = fDAs * FDDMIN
SaAs = fSaAs * SAin
AsP = As/Ascor * KWAP
absRAs = KAsabs * cAs
cAs = (As/Ascor)/(RLv/RLvcor)
As = INTEG(DAs,IAs)
```

Lipids (Fl,Fa in moles)

```
CONSTANT FDLiFl = 1.8,FDLiCh = 0.133,FDFaFl = 3.0
DFl = FDFl + FDFl1 – FlMi – FaP
FDFl = fDLi * FDDMIN/MWFlLi * FDLiFl
FDFL1 = FDFAT * FDDMIN * FDFaFl/MWFlFa
FlMi = MiG * FlMiG
```



```
FaP = KWAP * Fl/Flcor
Fl = INTEG(DFl,IFl)
```

Volatile fatty acids and lactate (RAc,RPr,RBu,RLa in moles)

'Rate constants for absorbtion of all VFA may not be equal as assumed here. KabsLa is set low to allow maximal La fermentation and create acidosis if desired, but the rate constants must be considered to be ill-defined.'

```
CONSTANT KabsAc = 10.5,KabsPr = 10.5,KabsBu = 10.5,KabsLa = 0.1
'ACETATE'
DRAc = FDFvAc + CsAc + RAaAc + RLaAc – absRAc – RAcP
FDFvAc = fDAc * FDDMIN/MWAc
CsAc = CsFv * CsFvAc
RLaAc = RLaFv * LaAcAc
CsFvAc = ScAc * fScCs + StAc * fStCs + HcAcAc * fHcCs + CeAcAc * fCeCs
fScCs = ScTCs/Csin
fStCs = (StCs + HaCs)/Csin
fHcCs = HcCs/Csin
fCeCs = CeCs/Csin
RAaAc = AaFvAc * (RAaFv + (0.76 * FDNnAm))
absRAc = KabsAc * RAc/RAccor
cRAc = (RAc/RAccor)/(RLv/RLvcor)
RAcp = (RAc/RAccor) * KWAP
RAc = INTEG(DRAc,IRAc)
MPAc = (RAc/RAccor)/TVFA
'PROPIONATE'
DRPr = CsPr + RAaPr + RLAPr – absRPr – RPrP CsPr = CsFv * CsFvPr
RLaPr = RLaFv * LaPrPr
CsFvPr = ScPr * fScCs + StPr * fStCs + HcPrPr * fHcCs + CePrPr * FCeCs
RAaPr = AaFvPr * (RAaFv + (0.76 * FDNnAm))
RPrp = (RPr/RPrcor) * KWAP
cRPr = (Rpr/RPrcor)/(RLv/RLvcor)
absRPr = KabsPr * RPr/RPrcor
RPr = INTEG(DRPr,IRPr)
MPPr = (RPr/RPrcor)/TVFA
'BUTYRATE'
DRBu = CsBu + RAaBu + FDFvBu – absRBu – RBup
CsBu = CsFv * CsFvBU
CsFvBu = ScBu * fScCs + StBu * fStCs + HcBuBu * fHcCs + …
CeBuBu * fCeCs
RAaBu = AaFvBu * (RAaFv + (0.76 * FDNnAm))
FDFvBu = fDBu * FDDMIN/MWBu
absRBu = KabsBu * RBu/RBucor
RBuP = (RBu/RBucor) * KWAP
cRBu = (RBu/RBucor)/(RLv/RLvcor)
RBu = INTEG(DRBu,IRBu)
MPBu = (RBu/RBucor)/TVFA
'LACTATE'
CONSTANT KLaFv = 0.5
DRLa = CsLa + FDFvLa – RLaP – absRLa – RLaFv
CsLa = CsFv * CsFvLa
CsFvLa = ScLa * fScCs + StLa * fStCs $'assumes no Hc,Ce,Aa, go to La'
FDFvLa = FDDMIN * fDLa/MWLa
RLaP = (RLa/RLacor) * KWAP
```

```
cRLa = (RLa/RLacor)/(RLv/RLvcor)
RLaFv = kLaFv * CMiWA * RLa/RLacor
absRLa = RLa * KabsLa/RLacor
RLa = INTEG(DRLa,IRLa)
```

(h) Microbial growth and passage

'Early dynamic models of rumen digestion such as those of Waldo et al. *(1972) and Nolan (1975) were restrictive, in that they considered either carbohydrate fermentation and passage alone or nitrogen metabolism alone. As a result, when applying the models of carbohydrate fermentation and passage, an implicit assumption was that nitrogen availability was adequate; when models of nitrogen metabolism were used, the implicit assumption was that energy (from carbohydrate) was not limiting or limiting to a constant extent. Yet these models were very useful in describing and comparing individual data sets, e.g. do these diets differ because fermentation rates differ or because passage rates differ, etc. When interactions occur across diets or between energy and nitrogen availabilities, microbes must be considered explicitly in the model, because effects of nitrogen availability upon carbohydrate fermentation are mediated, in large part, via effects upon microbial growth and vice versa.'*

'There are about 20 prominent microbial species in the rumen. Interactions among these are very complex and have not been modeled, probably because of an untested presumption that current concepts and data are not adequate to support such a modeling analysis. Lacking a detailed modeling analysis of the rumen ecosystem to guide the formulation of simplified representations of microbial functions in models of the ruminant digestive process, a number of alternative approaches to depict microbial growth and function have been proposed. The simplest approach was to consider the microbes in aggregate as one multifunctional group (Beever et al., *1981; France* et al., *1982). The assumption that underlies this approach is that the primary cause of variation in the microbial population is diet composition. Further, this approach implies that the primary or most important result of changes in the microbial population at this level of aggregation is the effect upon products of fermentation. The analyses of Murphy* et al. *(1982a) were undertaken to support implementation of this approach. A problem associated with this approach has been that when a highly available carbohydrate source such as starch was provided in the diet, the increase in microbial mass results in unacceptably high rates of hemicellulose and cellulose digestion (Baldwin* et al., *1987b). This led to development of the equations presented above to largely restrict the capacity for hydrolysis of starch, hemicellulose and cellulose to microbes that grew in association with each respective substrate. This approach also produces a lag (while associated microbes proliferate) in hydrolysis of insoluble substrates similar to that which occurs in reality.*

This current representation is simpler than the conceptually similar approach utilized by Baldwin et al. *(1977) and Murphy* et al. *(1986), where four differential equations for each insoluble substrate were required. With this number of equations, parameter values could not be defended on the basis of available data. A third approach, which was utilized by Baldwin* et al. *(1970) and more recently by Fox* et al.

(1988) and Beever et al. *(1981), is to explicitly subdivide the microbial population into groups such as those that ferment soluble carbohydrates, starch and holocellulose. When associated and free populations of these groups are represented, rigorous parameterization, again, becomes a problem. An associated problem discussed by Baldwin* et al. *(1970) was deciding what proportion of hydrolytic products formed from particulate substrates are fermented by the amylolytic and cellulolytic populations and what proportion by the soluble carbohydrate fermenters. Also, specification of a specific set of stoichiometric coefficients for each of the three sub-groups is not adequate, because the mix of microbes in each group vary with diet. The analyses of Murphy* et al. *(1982a) and other data discussed in Chapter 8 clearly indicate that this is true. In the face of these uncertainties and complexities, we believe that the modified single population represented herein is in keeping with the degree of aggregation required by our objectives and our ability to parameterize the equations based upon available data. Changes or additions will be required when data and modeling analyses indicate these are needed. This necessity has not yet been encountered.'*

'Estimates of microbial growth require, at a minimum, specification of microbial composition (a known variable considered as a constant herein), precursors of each component, ATP yields from fermentation, microbial maintenance requirements and factors that influence the net efficiency of microbial growth.'

'MICROBIAL COMPOSITION (kg/kg)'

'NOTE: Organic Matter only. These values are from Reichl and Baldwin (1975).'

```
CONSTANT MiPiPi = 0.572,MiNnNn = 0.095,MiHaHa = 0.212,MiLiLi = 0.121
'Lipid composition in mole/mole'
CONSTANT MiLiFa = 1.2,MiLiBu = 0.5,MiLiPr = 1.0,MiLiCh = 0.8,MiLiG1 = 0.5
MWMiLi = 0.632 $ HMiLi = 4.53 * F1
```

'Two alternative sets of stoichiometric factors for growth are considered: G1 in which amino acids and peptides are not used; and, G2 in which up to one-half of microbial protein can be derived from amino acids and peptides dependent on their availabilty.'

```
CONSTANT CsMiG1 = 6.133,AmMiG1 = 7.33,HyMiG1 = 2.71,CdMiG1 = 0.518
CONSTANT FlMiG = 0.23
CONSTANT CsMiG2 = 2.133,AmMiG2 = 1.12,KYATAa = 0.0001,AaMiG2 = 4.97, ...
HyMiG2 = - 0.42,CdMiG2 = - 0.05
G1 = 1.0 - G2
G2 = 0.5/(1.0 + KYATAa/cRAa)
PROCEDURAL (MiMaAd = RpH) $ 'Effect of pH on the microbial maintenance requirement.'
MiMaAd = 20 $ 'moles/kg/day'
IF(RPH.GE.6.2) GO TO 26
IF(RPH.LE.5.4) GO TO 25
MiMaAd = MiMaAd + (MiMaAd * ((0.8 - (RPH - 5.4))/0.8))
GO TO 26
25.. MiMaAd = 40
26.. CONTINUE
END                                    $ 'OF PROCEDURAL'
```

```
CONSTANT RYATP = 0.013,KFgAm = 0.0012,LaFvAT = 1.0
CONSTANT KFATFg = 0.03
```

'Microbial growth (MiG) is a function of ATP derived from fermentation (ATPF), ATP used in maintenance functions (ATPM) and modifiers of the efficiency of use of ATP available for growth including YATP, which is a function of amino acid availability, ammonia concentration and dietary fat.'

```
DMi = MiG – MiP
MiG = ATPG * YATP * FgAm * FgFa
ATPG = ATPF – ATPM
ATPF = CsFv * CsFvAT + RAaFv * AaFvAT + 0.76 * FDNnAm * AaFvAT + RLaFv *
       LaFvAT
ATPM = Mi/Micor * MiMaAD
FgAm = 1.0/(1.0 + KFgAm/cAm)
FgFa = 1 + (FDFAT/fDLi * KFATFg)
YATP = 0.012 + RYATP/(1.0 + KYATAa/cRAa)
YATPAP = MiG/ATPF
MiP = SpMiP + WAMiP
SpMiP = KSPP * SpMi
WAMiP = KWAP * WAMi
```

'Distribution of microbes among water, Sp and Lp is dependent upon fractions of total dry matter in each pool.'

```
LpMi = ((Lp/Lpcor)/(RDM – Mi)) * Mi/Micor
SpMi = (Sp/(RDM – Mi)) * Mi/Micor
WAMi = (Mi * SOLDM/(RDM – Mi))/Micor
cMiSp = SpMi/Sp
cMiWa = WaMi/SOLDM
Mi = INTEG(DMi,iMi)
```

(i) Methane production

```
CONSTANT AaFvHY = 1.14
   DTCH4 = DDCH4
   DCsFvH = CsFvAc * 2.0 – CsFvPr * 1.0 + CsFvBu * 2.0
   DCsHy = CsFv * DCsFvH
   DRAaHy = RAaFv * AaFvHy
   DHyMi = HyMiG1 * G1 + HyMiG2 * G2
   DHyFlF = FDFl * 2.0
   DTHy = DCsHy + DRAaHy – DHyMi – DHyFlF + 2.0 * RLaAc – RLaPr
   DDCH4 = DTHy/4.0
```

(j) Lower gut digestion (LG) equations are basically defined by digestion and fermentation coefficients input by user

```
CONSTANT LGDCHa = 0.7,DCMiPi = 0.75,DCMiLi = 0.7,LGDCHb = 0.1
CONSTANT LGDCPi = 0.4,LGDCAs = 0.85,LGDcAi = 0.10,LGDCFa = 0.9
   LGHaGl = HaP * LGDCHa/MWSt
   MiGl = MiP * MiHaHa * LGDCHa/MWSt
   MiAa = MiP * MiPiPi * DCMiPi/MWPi
   MiLiDg = MiP * MiLiLi * DCMiLi/MWMiLi
   MiFa = MiLiDg * MiLiFa
```



```
LGFaDg = LGDCFa * FaP
MiBu = MiLiDg * MiLiBu
MiPr = MiLiDg * MiLiPr
MiLGl = MiLiDg * MiLiGl
MiCh = (MiP * MiLiLI/MWMiLi) * MiLiCh
LGHcFv = HcP * LGDChb/MWHc * 0.833
LGHcAc = LGHcFv * HcAcAc
LGHcPr = LGHcFv * HcPrPr LGHcBu = LGHcFv * HcBuBu
LGCeFv = CeP * LGDChb/MWCe
LGCeAc = LGCeFv * CeAcAc
LGCePr = LGCeFv * CePrPr
LGCeBu = LGCeFv * CeBuBu
LGPiAa = PiP * LGDCPi/MWPi
LgAs = LgDcAs * AsP
LgAi = LgDcAi * OtP * fDAi/fOt
```

(k) Computation estimates of rumen and overall digestion coefficients and energetic relationships

```
'FECES'
   FEHa = HaP * (1.0 – LGDCHa)
   FEHb = HbP * (1.0 – LGDCHb)
   FEHc = HcP * (1.0 – LGDCHb)
   FECe = CeP * (1.0 – LGDCHb)
   FMiPi = MiP * MiPiPi * (1.0 – DCMiPi) $KG.
   FMiNn = MiP * MiNnNn
   FMiLi = MiP * MiLiLi * (1.0 – DCMiLi)
   FEFa = FaP * (1 – LGDCFa) * MWFl
   FEPi = PiP * (1.0 – LGDCPi)
   FEASH = AsP * (1.0 – LGDCAs) + OtP * fDAi/fOt * (1.0 – LgDcAi)
   FEMiHa = MiP * MiHaHa * (1.0 – LGDCHa)
   FELg = OtP * fDLg/fOt
   FEPiT = FMiPi + FMiNn + FEPi
   FECh = ((fDLi * FDDMIN/MWFDLi) * FDLiCh) * MWCh + MiCh * DCMiLi * MWCh
   FEOM = FEHa + FEHb + FEPiT + FMiLi + FELg + FECh + FEMiHa + FEFa
   FEENG = (FEHa * 4.154 + FEHb * 4.154 + (FMiPi + FEPi) * 5.7 + FMiLi * 7.2 + …
   FELg * 8.3 + FECh * 3.31 + FMiNn * 5.7 + FEMiHa * 4.154 + FEFa * 9.53) * F1
   FEDM = FEOM + FEASH
   SOLDMP = SOLOMP + AsP
   TOMP   = SOLOMP + HaP + HbP + PiP + OtP * fLgOt
   TTOMP  = TOMP + MiP $ 'RUMEN DIGESTION COEFFICIENTS'
   RDCOM  = 1.0 – TOMP/FDOMIN $ 'FOR TRUE ORGANIC MATTER'
   RDCOMa = 1.0 – TTOMP/FDOMIN $ 'FOR APPARENT ORGANIC' MATTER
   TStin = FDDMIN * FdSt
   DCHa = (TStin – FEHa)/TStin
   DCHb = (Hbin – FEHb)/Hbin
   DCLg = ((fDLg * FDDMIN) – FELg)/(fDLg * FDDMIN)
   DCPRT = (TPRTin – FEPiT)/TPRTin
   DCOM   = (FDOMIN – FEOM)/FDOMIN $ 'DIGESTION COEFFICIENTS'
   DCDM   = 1.0 – FEDM/FDDMIN $ 'FOR: ORGANIC AND DRY MATTER'
   'Computation of digestion coefficients for energy and energy terms.'
   FDGEin = FDGE * FDDMIN + INFPRT * 5.7
```

```
AccGEI = INTEG(FDGEin,1.0E – 8)
TDE = absE/FDGEin
appDE = (FDGEIN – FEENG)/FDGEIN $ 'APPARENT DIGESTIBLE ENERGY'
DEI  =  FDGEin – FEENG $ 'DIGESTIBLE ENERGY INTAKE'
DE   =  DEI/FDDMin $ 'DIGESTIBLE ENERGY'
AccDEI = INTEG(DEI,1.0E – 8)
CH4E =  DTCH4 * HCH4 $ 'APPARRENT AND CORRECTED'
EUR  =  DUREA * HcUR $ 'METABOLIZABLE ENERGY'
MEI = (FDGEin – CH4E – EUR – FEENG)
AccMEI = INTEG(MEI,1.0E – 8)
ME1 = MEI/FDDMIN
GE = FDGEin/FDDMIN
HFERM = FDGEin – absE – FEENG – CH4E – EUR
corMEI = MEI – HFERM
corME = corMEI/FDDMIN
```

16.3.5 Interface of digestion and animal elements

'This section computes the absorbtion of nutrients from gut in moles. This is the input to the animal model.'

```
absGl = LGHaGl + CsP + MiGl + MiLGl
absAa = MiAa + LGPiAa + RAaP + INFPRT/0.110
absAc = absRAc + LGHcAc + LgCeAc + RAcP
absPr = absRPr + MiPr + LGHcPr + LgCePr + RPrP
absBu = absRBu + LGHcBu + LgCeBu + MiBu + RBuP
absAm = absRAm
absFa = (MiFa + LGFaDg) * MWFl/MWFa
```

'The ratio MWFl/MWFa converts stearate (Fl) from gut to palmitate in animal.'

```
absAs = absRAs + LgAs + LgAi absLa = absRLa + RLaP
absAcE = absAc * HCAc
absPrE = absPr * HCPr
absBuE = absBu * HCBu
absFaE = absFa * HCFa
absAaE = absAa * HCAa
absGlE = absGl * HCGl
absLaE = absLa * HCLa
AbsE = absAcE + absPrE + absBuE + absFaE + absAaE + absGlE + absLaE
```

16.3.6 Dynamic elements of the animal submodel

'A basic premise underlying formulation of the animal element of the lactating cow model was that efficiencies of utilization of the specific absorbed nutrients inherently differ as discussed in Chapters 5 and 6. Thus, in keeping with our modeling objective, it was essential the animal submodel consider specific chemical entities and their respective rates of utilization for alternative processes explicitly (Baldwin et al., *1987a).'*

'A number of simplifying assumptions were made to keep the model simple and achieve reasonable solution speeds with then current computers. All absorbed

butyrate was assumed to be oxidized. Ketone bodies are not represented and, thus, the model cow cannot become ketotic (we have a version in which ketosis can occur). Minerals and micronutrients are not represented, and thus their availability is assumed to be adequate. When this is not so, the model will fail to simulate experimental data. Similarly, amino acids are considered in aggregate, with the result that responses to experimental manipulations of the balance of amino acids supplied, e.g. administration of rumen-protected lysine and methionine, cannot be simulated (again, there is a current version with this capacity). State variables, transaction and reference fluxes are presented in Fig. 16.2. Bases for initial calculations presented as comments in the model refer to the initial model version for the reference cow (Chapter 13). Some drift from these conditions has occurred over the years but in general, original and current values are quite close. As above, reasons for significant changes from the original and added comments are presented in quotes.'

*'A significant change from the original was changing many V_{max} specifications from constants to variables ($V_{max}F$ * $EBW^{0.75}$) so as to allow for a range of initial empty body weights.'*

(a) Mammary gland elements

'Several inputs to this section were presented and discussed as initial conditions in the initial section.'

```
CONSTANT MLKINT = 1.0,MLTM = 1.0 $ 'Milking'
PROCEDURAL (KMILK = MLKINT,MLTm,TIME)
KMILK = 0.0
IF(AMOD(TIME,MLKINT).LE.MLTm)GO TO 50
GO TO 51
50.. KMILK = 2.91/UMLKcr
GO TO 51 51.. CONTINUE
END                                    $ 'OF PROCEDURAL'
DLHOR = – KLHOR * LHOR $ 'LACTATION HORMONE'
LHOR = INTEG(DLHOR,ILHOR)
DUENZ = Usyn – Udeg $ 'UDDER ENZYMES'
Usyn = VUsyn * Ucells * LHOR * BST/(KUsyn + LHOR * BST)
Udeg = UENZ * (KUdeg + KUdegM * ((UMave/KMdeg) * * THETA5/(1.0 + ...
UMave/KMdeg) * * THETA5))
DUMave = TaveM * (UMILK – UMave) $ 'RETAINED MILK EFFECTS'
UMave = INTEG(DUMave,IUMave)
KMinh = (MLKmax – UMILK)/(MLKmax – UMILK + KMLKI)
UENZ = INTEG(DUENZ,IUENZ)
```

(b) Anabolic and catabolic hormones

```
AHOR = (cGl/IcGl) * * theta2
AHOR1 = (cGl/IcGl) * * theta4
CHOR = (IcGl/cGl) * * theta3
CHOR1 = (IcGl/cGl) * * theta4
```

'Metabolic hormones such as insulin, glucocorticoids, glucagon, catecholamines etc., clearly fulfil a central role in the coordination of animal metabolism in rum

nants as well as non-ruminant species. Specific roles for many of the metabolic hormones have been well studied in other species, particularly rodents, but not ruminants. Studies with ruminants have been adequate with some notable exceptions, to assure that mechanisms of action of the metabolic hormones are the same as those observed in rats, but also have shown that the magnitude of responses in ruminants are very low relative to rodents. For example, respective maximum responses of ruminant adipocytes to insulin, glucagon, and catecholamines are 1.3-, 2.0- and 2.0-fold as compared to 4.0-, 8.0- and 6.0-fold in rodents (Yang and Baldwin, 1973a,b; Vernon, 1980). Acute effects of glucagon upon rates of gluconeogenesis in ruminant hepatocytes were marginal (Looney et al., *1987) and chronic effects of adrenalectomy on rates of gluconeogenesis in sheep liver were absent (Ely and Baldwin, 1976), while gluconeogenic responses in rats to glucocorticoids and gluconeogenesis are very prominent. Since rates of gluconeogenesis are maximal in fed ruminants and in fasted rats, one might expect species differences. Effects of glucocorticoid insufficiency on rat mammary glands are highly significant (Louis and Baldwin, 1975) and absent in sheep mammary glands (Ely and Baldwin, 1976).'*

'These observations clearly indicate that additional data on the actions of metabolic hormones in ruminants are required, as current data are not adequate to support the development of detailed models of metabolic hormone actions in ruminants and, certainly, require that their actions be represented very simply in ruminant metabolism at the whole-animal level. These observations led to two decisions about how metabolic hormones function in this model. The first was that the metabolic hormones be represented in two aggregate groups – anabolic (AHOR) and catabolic (CHOR). The second was that both homeostatic and homeorhetic processes operate to assure that adequate nutrient supplies be available to tissues for performance of their functions. Glucose is a prominent indicator of such adequacy and thus could be used to drive the relative signals for anabolic and catabolic responses as in the equations below.'

(c) Lipid metabolism (Fa,Ts)

'Inputs to the storage triacylglyceride pool (Ts) are fatty acid esterification (FaTsF * FaTsTS = 6 * 0.33 = 2.0) and lipogenesis from acetate (AcTs * AcTsTS = 16 * 0.042 = 0.667). Output is lipolysis (TsFaF = 2.667). Inputs to the fatty acid plus triacylglyceride pool (Fa) are absorption (absFa = 1.0) from gut and lipolysis (TsFaF * TsFaFA = 2.667 * 3 = 8.0). Outputs are fatty acid (re)esterification (FaTsF = 6.0), incorporation into milk fat (FaTmV = 1.8) and oxidation (FaCd = 1.2).'

'The current equation for TsFa differs from the original, where energy balance was a major effector of lipolytic rates. The change was forced by the observation that in early lactation, when simulated, cows were in severe negative energy balance; lipolytic rates were too high, which resulted in elevated blood lipids and uptake by the udder. As a result, milk fat percentages were elevated above normal, thus exacerbating the negative energy balance. In the current equation, catabolic hormones and thyroxin can elevate the V_{max} *for lipolysis. As in the original equation the high*

value of THETA1 (= 5.0) assures that the concentration of triglyceride (cTs) do not become limiting until about 80% of Ts has been mobilized. The added ter cFa/k1TsFa represents a negative feedback of fatty acids on lipolysis. Several obse vations support this effect.'

'cFa is 0.5E – 3 and cGl is 3.0E – 3. KFaTsF was set at 1.67E – 4 to make cF close to saturating and K1FaTs at 2.0E – 3 to make the reaction responsiv to Gl changes. Aggregation confounds KFaTmV and VFaTmV so these we set to produce 1/2 V_{max} in the reference state.'

```
CONSTANT TgFaFa = 3.0,AcAcTs = 24.0,VTsFaF = 5.0E – 2,KTsFaF = 0.2
CONSTANT theta1 = 5.0,MWTs = 0.806
CONSTANT KFaTsF = 5.0E – 4,K1FaTs = 2.0E – 3,K1TsFa = 5.0E – 4
CONSTANT VFaTsF = 0.113,KFaTmV = 5.0E – 4,VFaTmV = 0.75E – 3
CONSTANT FaTgTg = 0.333,AcTgTg = 0.041667,K1FaTm = 1.5E – 3
CONSTANT theta2 = 2.0,theta3 = 2.0,theta4 = 1.0,P1 = 2.0
CONSTANT EXP10 = 2.0
WTCYTF = 15.0/500 * bwf

'STORAGE TRIACYLGLYCEROL METABOLISM'
DTsF = FaTsF1 + AcTsF1 – TsFaF
TsFaF = VTsFaF * (EBW * * 0.75) * CHOR1 * T3/(1.0 + (cFa/K1TsFa) * * EXP10...
        + (KTsFaF/cTs) * * theta1)
cTs = TsF/WTF
FaTsF1 = FaTsF * FaTgTg
AcTsF1 = AcTsF * AcTgTg
WTF = WTCYTF + MWTs * TsF
DWTTsF = DTsF * MWTs
TsF = INTEG(DTsF,ITsF)
'PLASMA LIPID METABOLISM'
DFa = absFa + TsFaF1 – FaTsF – FaTmV – FaCd
FaTsF = VFaTsF * (EBW * * 0.75)/(1.0 + KFaTsF/cFa + K1FaTs/(AHOR * cGl))
cFa = Fa/VFA
TsFaF1 = TsFaF * TgFaFa
FaTmV = (VFaTmV * UENZ * KMinh)/(1.0 + KFaTmV/cFa + K1FaTm/cGl)
Fa = INTEG(DFa,IFa)
```

(d) Acetate metabolism (Ac)

'Inputs are from absorbtion (absAc = 65.9) and gluconeogenesis (AaGlV AaAcAc = 4 * 0.6 = 2.4). Output is oxidation (AcCd = 35.5) and lipogene in adipose and mammary (AcTsF = 16.0, AcTmV = 16.8). AaAcAa set at (to replace 0.27 KB on an equal –P basis. Must correct final output of Cd f excess produced by this compromise. Respective Ks values for Ac and Gl adipose and mammary are similar at 1.5–2.0 and 0.8–1.0 mM. Thus set 1.8E – 3 and 1.0E – 3 for both tissues. Chronic regulation of adipose lipoger capacity (VAcTsF) was included to stimulate effects of energy balan throughout lactation.'

```
CONSTANT K1VAct = 0.06,K2VAcT = 0.268, IVAcTs = 0.35
DVAcTs = K1VAcT * AHOR1 – K2VAcT * VAcTsF
VAcTsF = INTEG(DVAcTs,IVAcTs)
CONSTANT KAcTsF = 1.8E – 3,VAcTmV = 10.0E – 3...
```

```
K1AcTs = 1.0E – 3,AaGlAc = 0.6,KAcTmV = 1.8E – 3,K1AcTm = 1.0E – 3
DAc = absAc + AaAcV1 – AcTsF – AcTmV – AcCd
AaAcV1 = AaGlV * AaGlAc
AcTsF = Vmax/(1.0 + KAcTsF/cAc + K1AcTs/(AHOR * cGl))
Vmax = VAcTsF * (EBW * * 0.75)
cAc = Ac/VAc
AcTmV = VAcTmV * UENZ * KMinh/(1.0 + KAcTmV/cAc + K1AcTm/cGl)
Ac = INTEG(DAc,IAc)
'MILK FAT SECRETION (UTm, DMLKTm,TMLKTm)'
CONSTANT MWTm = 0.806
DUTm = (AcTmV1 + FaTmV1) * MWTm – DMLKTm
DMLKTm = UTm * KMILK
UTm = INTEG(DUTm,IUTm)
TMLKTm = INTEG(DMLKTm,1.0E – 8)
```

(e) DNA accretion, not a variable in original model

'Equations adapted from DiMarco and Baldwin (1989).'

```
CONSTANT ExpB2 = 1.19,KDNAb = 7.36E – 4,ExpV2 = 0.96,KDNAv = 1.7E – 4...
BDNAmx = 0.112, VDNAmx = 0.110
DBDNA = (KDNAb * * ExpB2) * ((BDNAmx – BDNA)/BDNAmx)
DVDNA = (KDNAv * * ExpV2) * ((VDNAmx – VDNA)/VDNAmx)
BDNA = INTEG(DBDNA,IBDNA)
VDNA = INTEG(DVDNA,IVDNA)
```

(f) Amino acid and nitrogen metabolism

'Amino acid metabolism (Aa) including protein turnover in Body (Pb) and Viscera (Pv). Inputs to Aa are absAa (12.6), PbAa (10.0) and PvAa (8.2). The interspecific protein degradation at rate of 18 g/$BW^{0.75}$ from Reeds (1989) indicates a rate of 2.0 kg/day or (/0.110) 18.2 moles/day in the reference animal. Data (Sainz *et al.*, 1986) on lactating rats indicate this estimate may be low. Outputs are AaPbB (10), AaPv (8.2), AaPm (8.6) and gluconeogenesis (AaGlV = 4.0). Biosynthetic reactions set at 1/2 V_{max} in reference state. Capacity for AaGlV is very high (five times) relative to flux in the fed (reference) state and was set there. Computation of mass in B and V assumes that protein is 25% dry matter (fractional dry weight = fdwt) and that remaining weight is constant (otwtB,otwtV). KPbAaB and KPvAaV were adjusted 05/01/91 to make equations functions of Pb and Pv rather than cPb and cPv. VAaGlV was also scaled to body size (BWF).'

'Provisions for energy use associated with pregnancy were not included in the original model. When these were added to energy requirements as in RFEED8, a provision for removal of amino acids for protein accretion at the rate of 0.05 of the fetal ME requirement (Aapreg) was added.'

```
CONSTANTVAaPbB = 300,VAaPvV = 200,KAaPbB = 2.5E – 3,KAaPvV = 2.5E – 3 ...
VAaPmV = 2.89E – 3,VAaGlV = 0.228,KAaGlV = 10.0E – 3,KPbAaB = 0.030 ...
KPvAaV = 0.090,fDWT = 0.25,AaGlUr = 0.62,KAaPmV = 2.1E – 3 MWPb = 0.110,VSIZf
        = 80.0
```



```
OtWTB = 103.6/500 * BWF
OtWTV = 22.2/500 * BWF
```

Amino acid metabolism and protein turnover

```
DAa = absAa + PbAaB + PvAaV – AaPbB – AaPvV – AaPmV – AaGlV – SaPsAa –
Aapreg
DPb = AaPbB – PbAaB
DPv = AaPvV – PvAaV
PbAaB = KPbAaB * Pb
PvAaV = KPvAaV * Pv
cPb = Pb/WTB
cPv = Pv/WTV
WTB = Pb * MWPb/fDWT + OtWTB DWTB = DPb * MWPb/fDWT
WTV = Pv * MWPb/fDWT + OtWTV
DWTV = DPV * MWPb/fDWT
AaPbB = VAaPbB * BDNA/(1.0 + KAaPbB/(AHOR * cAa))
AaPvV = VAaPvV * VDNA/(1.0 + KAaPvV/(AHOR * cAa))
PbFsR = AaPbB/Pb
PvFsR = AaPvV/Pv
PbFdR = PbAaB/Pb
PvFdR = PvAaV/Pv
AaPmV = VAaPmV * UENZ * KMinh/(1.0 + KAaPmV/cAa)
AaGlV = VAaGlV * (EBW * * 0.75)/(1.0 + KAaGlV/(CHOR * cAa))
cAa = Aa/VAa
Aapreg = FMEREQ * 0.05/HcAa
Pv = INTEG(DPv,IPv)
Pb = INTEG(DPb,IPb)
Aa = INTEG(DAa,IAa)
'AMMONIA AND UREA METABOLISM'
CONSTANT AmUrUr = 0.5,KPUNU = 857.1
DPUN = AaUr + AmUr – PUNRAm – SaNRAm – DUREA
AaUr = AaGlV * AaGlUr
AmUr = absAm * AmUrUr
PUNRAm = PUNAm * AmUrUr
SaNRAm = SaNnAm * AmUrUr
DUREA = KPUNU * cPUN
PUN = INTEG(DPUN,IPUN)
'MILK PROTEIN SECRETION (UPm, DMLKPm,TMLKPm)'
CONSTANT MWAa = 0.133
DUPm = AaPmV * MWAa – DMLKPm
DMLKPm = UPm * KMILK
UPm = INTEG(DUPm,IUPm)
TMLKPm = INTEG(DMLKPm,1.0E – 8)
```

(g) Glucose metabolism (Gl)

'Entries are from propionate (9.84), lactate (4.05), glycerol (3.59), Aa (1.8 and absorption (4.7). Outputs are to lactose (8.3); the glycerol moiety triacylglycerol (0.95), pentose cycle (1.47) and TpCd (2.04/2) in V; to Cd (4 and lactate (La, 4.9/2) in B, and to pentose cycle (2.8/2), triacylglycer (2.667/2), La (3.2/2) and TpCd ((1.4 + 0.47)/2) in adipose tissue.'

'Reported (Forsberg *et al.*, 1985) $K_{Gl,LmV}$ for Gl for lactose synthesis is 8–10 mM so set at 9.0E – 3. $NADPH_2$ required from the pentose cycle for fatty acid synthesis is calculated in terms of moles Gl (GlHy) used, since reaction rate is computed as acetate used per Ac incorporated. Stoichiometry for pentose cycle used is Gl to 3Cd + 6$NADPH_2$ + Tp. Thus, the stoichiometric coefficient (GlGlHy) is calculated as (1.75 $NADPH_2$/AcFa)/6$NADPH_2$ per glucose used (= 0.292). These must be multiplied by the fraction of $NADPH_2$ generated via the pentose cycle specified as input for that tissue (fGlHyF and fGlHyV) and AcTs flux to get actual pentose cycle flux. Related calculations are of ATP equivalents of amount of $NADPH_2$ generated in the tricarboxylic acid cycle by the NADP-linked isocitrate dehydrogenase and of the reduction in oxygen consumption associated with this. These are in the oxidative metabolism section. In adipose tissue, GlTpF was set to provide Tp in excess of that required for fatty acid esterification. This accommodates the possibility that Tp generation via GlHy can be less than TpTs, and provides sufficient Tp for oxidation (TpCd) and conversion to lactate (La) as has been observed in this tissue. Lactate from B and F are quantitatively converted to Gl in V. *In accord with concepts presented in Chapter 4, glycerol and lactate are considered to be zero pools in this section.'*

```
CONSTANT AaGlGl = 0.47,PrGlGl = 0.5,LaGlGl = 0.5,GyGlGl = 0.5...
VGlLmV = 3.9E – 3,KGlLmV = 3.0E – 3,VGlTpF = 3.78E – 2,KGlTpF = 3.0E – 3,...
VGlTpV = 9.46E – 3,KGlTpV = 3.0E – 3,fLaCdF = 0.226,KGlLaB = 1.5E – 3,...
VGlLaB = 4.61E – 2,fLaCdB = 0.246,GLGlHy = 0.292,pGlHyF = 0.6,...
pGlHyV = 0.6,fPrGl = 0.7,TgGyGy = 1.0,GlLaLA = 2.0,GlHyTP = 1.0,...
GlTpTp = 2.0,TpTpTs = 1.0,GlGyGy = 2.0,KAaLmV = 2.0E – 3,...
DGl = upGl + AaGlV1 + PrGlV1 + LaGlV1 + GyGlV1 – GlLmV – ...
GlHyF – GlHyV – GlTpF – GlTpV – GlLaB – GlCd
upGl = 0.10 * absGl
AaGlV1 = AaGlV * AaGlGl
PrGlV1 = PrGlV * PrGlGl
PrGlV = absPr * fPrGl
LaGlV1 = (LaGlF + LaGlB + RLaGl) * LaGlGl
RLaGl = absRLa + RLaP + GGlLa
GGlLa = 0.90 * absGl * GlLaLa
GyGlV = (TsFaF + FaTmV1) * TgGyGy
GyGlV1 = GyGlV * GyGlGl
GlLmV = VGlLmV * UENZ * KMinh/(1.0 + KGlLmV/cGl + KAaLmV/cAa)
cGl = Gl/VGl
GlHyF = AcTsF * fGlHyF * GlGlHy
GlHyV = AcTmV * fGlHyV * GlGlHy
```

'pGlHyF and pGlHyVb are not constants and should become dependent variables when appropriate equation forms are deduced using tissue models.'

```
fGlHyF = pGlHyF
fGlHyV = pGlHyV
GlTpF = VGlTpF * (EBW * * 0.75)/(1.0 + KGlTpF/cGl)
GlTpV = VGlTpV * (EBW * * 0.75)/(1.0 + KGlTpV/cGl)
GlLaB = VGlLaB * (EBW * * 0.75)/(1.0 + KGlLaB/cGl)
TpinF = GlHyF * GlHyTP + GlTpF1
GlTpF1 = GlTpF * GlTpTp
```



```
TpinV = GlHyV * GlHyTp + GlTpV1
GlTpV1 = GlTpV * GlTpTp
LainB = GlLaB1
GlLaB1 = GlLaB * GlLaLa
TpLaF = TpinF – TpTsF
TpCdV = TpinV – TpTmV
TpTsF = (FaTsF1 + AcTsF1) * TPTpTs
TpTmV = (FaTmV1 + AcTmV1) * TPTpTs
AcTmV1 = AcTmV * AcTgTg
FaTmV1 = FaTmV * FaTgTg
LaCdF = TpLaF * fLaCdF
LaGlF = TpLaF – LaCdF GlGyT = (TpTsF + TpTmV) * GyGlGl
LaCdB = LainB * fLaCdB
LaGlB = LainB – LaCdB
Gl = INTEG(DGL,IGl)
'LACTOSE SECRETION (ULm, DMLKLm,TMLKLm) plus TOTAL MILK YIELD'
CONSTANT GlLmLm = 0.5,MWLm = 0.342,PCLm = 0.048
DULm = GlLmV * GlLmLm * MWLm – DMLKLm
DMLKLm = ULm * KMILK
DMILK = DMLKLm/PcLm
ULm = INTEG(DULm,IULm)
TMLKLm = INTEG(DMLKLm,1.0E – 8)
TVMLK = TMLKLm/PcLm
UMILK = ULm/PcLm
```

(h) Oxidative metabolism (Ox,Cd)

'Computations based on energy needs expressed as rate of ADP formatio (AtAd_), oxygen (Ox) uptake calculated from P/O ratio (PO), and Ac and F oxidation rates from ratios of Michaelis–Menten type equations assumin Vmaxs for oxidation of each are equal. *See Chapter 4 for details regardir oxidative metabolism and the treatment of ATP and ADP as zero pools.'*

```
CONSTANT GlCdAT = 38.0,AcCdAT = 10.0,FaCdAT = 129.0,GyGlAT = 2.0,...
PrCdAT = 18.5,TpCdAT = 20.0,LaCdAT = 18.0,TpLaAT = 2.0,GlLaAT = 2.0,...
BuCdAT = 25.0,HyAtAT = 3.0
CONSTANT AaPxAD = 5.0,GlHyAD = 1.0,GlTpAD = 2.0,LaGlAD = 3.0, ...
TpTgAD = 9.0,AcFaAD = 2.875,TcHyAD = 5.25,GlLmAD = 1.0,PrGlAD = 2.0,...
abGlAD = 1.0,abAaAD = 1.0
CONSTANT OxAcCd = 2.0,OxPrCd = 3.5,OxBuCd = 5.0,OxGlCd = 6.0,...
OxLaCd = 3.0,OxTpCd = 3.0,OxFaCd = 23.0,OxPrGl = 1.0
CONSTANT AcCdCD = 2.0,PrCdCD = 3.0,BuCdCD = 4.0,GlCdCD = 6.0,...
GlHyCD = 3.0, FaCdCD = 16.0,LaCdCD = 3.0,TpCdCD = 3.0
```

'Computation of effects of feed intake (absorbed energy) on basal energ expenditures. Absorbed energy is averaged (abEave) over 20 days (Tavab = 1/20). Absorbed energy factor (abEf) is expressed in units of metaboli body weight. *This implements concepts introduced in Chapter 6 that basal energ expenditures vary with feed intake.'*

```
CONSTANT TavabE = 0.05
DabEav = TavabE * (absE – abEave)
abEave = INTEG(DabEav,IabEav)
abEf = abEave/(EBW * * 0.75)
```

```
AtAd = AtAdB + AtAdF + AtAdV
AdAt = AdAtB + AdAtF + AdAtV
EBW1 = WTB + WTF + WTV
BW1 = EBW1 + RUMvol
```

ATP use and heat production in body (B)

'Energy expenditures in reference state expressed as ATP utilization are basal (294) and protein synthesis (50) for a sum of 344. Mandatory ATP generation from glucose because brain and kidney are in this element is GlLaB * GlLaAT (4.75 * 2.0 = 9.5) plus LaCdB * LaCdAT (4.6 * 18 = 82.8) for a sum of 92.3. Basal energy expenditures also vary with thyroid status.'

```
CONSTANT kbasB = 2.634,KNaB = 0.119,HYAcFa = 1.75,AaGlH = 0.554
AtAdB = basalB + AtAdB1
AtAdB1 = AaPbB * AaPxAD
basalB = (kbasB + KNaAtB) * wtB * * 0.75
KNaAtB = 0.8 + KNaB * T3 * abEf
AdAtB = AdAtB1 + AdAtB2
AdAtB1 = GlLaB * GlLaAT
AdAtB2 = LaCdB * LaCdAT
'Heat production in body'
basHtB = basalB * AtAdHt
AaPbHt = AtAdB1 * AtAdHt
MHtB = basHtB + AaPbHt
```

ATP use and heat production in adipose tissue (F)

'Energy expenditures (AtAdF = 169.2) are basalF (41.0); GlHyF (2.8); GlTpF (4.0); TpTsF * TpTsAD (2.667 * 9(6 ATP to form acyl CoA plus 3 for $NADH_2$ to reduce Tp) = 24); AcTsF * (tcHyAD * (1.0 – fGlHyF) = 16 * (5.25 * (1 – 0.6) + 2.875) = 16 * (2.1 + 2.875) = 79.6; tcHyAD is the cost of $NADPH_2$ from TCA cycle expressed in ATP per acetate (1.75 * 3 = 5.25); and, ATP cFa is cost in ATP/Ac converted to Fa * ((8Ac – 8AcCoA (= 16AtAd) + 7AcCoA – 7Mal – CoA * (= 7AtAd)) * 8 = 2.875). Oxidation of Tp yields 18.66 ATP and 6.4 ATP are generated in TpLaF. Reduction in oxygen uptake due to $NADPH_2$ generation in Tc is HYAcFa * (1.0 – fGlHyF) = 1.75 * 0.4 = 0.7 in this version.'

```
CONSTANT kbasF = 1.12,KNaF = 0.107
AtAdF = basalF + AtAdF1 + AtAdF2 + AtAdF3 + AtAdF4
basalF = (kbasF + KNaAtF) * wtF * * 0.75
KNaAtF = 0.3 + KNaF * T3 * abEf
AtAdF1 = GlHyF * GlHyAD
AtAdF2 = GlTpF * GlTpAD
AtAdF3 = TpTsF * TpTgAD
AtAdF4 = AcTsF * (tcHyAD * (1.0 – fGlHyF) + AcFaAD)
AdAtF = AdAtF1 + AdAtF2
AdAtF1 = TpLaF * TpLaAT
AdAtF2 = LaCdF * LaCdAT
'HEAT PRODUCTION IN ADIPOSE'
basHtF = basalF * AtAdHt
HtF2 = AtAdF2 * AtAdHt
HtF3 = AtAdF3 * AtAdHt – AcTsH4
MHtF = basHtF + HtF2 + HtF3
```


ATP use and heat production of viscera (V)

'Energy expenditures are basalV (339), TpTsV (* TpTsAD = 1.3 * 9 = 11.
AcTmV (16.8 * (see F) = 83.6), AaPrV (41), AaPmV (43), GlLmV (16.
GlHyV (1.47), GlTpV (0.4), LaGl (16.2), absGl (3.59) and absAa (12.6).'

'ATP use in fetal growth (AtAd16) set to equal 95% of ME intake f
gestation. Five percent was removed as Aa used for protein synthesis abo
Other nutrients are considered to be lost from the body in proportion
their availabilities and are accounted as heat losses in this scenario. Becau
of this, heat production in pregnancy is inflated by about 10% of FMERE

'ATP formation in viscera is from GyGlV (14.4), TpCdV (40.8), PrC
(156), BuCd (245).'

```
CONSTANT KbasV = 3.5,KNaV = 0.20,kidwrk = 0.378,hrtwrk = 0.096,...
reswrk = 0.3333,ATAmUr = 4.0
AtAdV = basalV + AtAdV1 + AtAdV2 + AtAdV3 + AtAdV4 + AtAdV5 + AtAdV6 + .
AtAdV7 + AtAdV8 + AtAdV9 + AtAd10 + AtAd11 + AtAd12 + AtAd13 + AtAd14 + .
AtAd15 + Atad16
basalV = (kbasV + KNaAtV) * wtV * * 0.75
KNaAtV = 3.2 + KNaV * T3 * fdomin
AtAdV1 = TpTmV * TpTgAD
AtAdV2 = AcTmV * (tcHyAD * (1.0 – fGlHyV) + AcFaAD)
AtAdV3 = AaPvV * AaPxAD
AtAdV4 = AaPmV * AaPxAD
AtAdV5 = GlLmV * GlLmAD
AtAdV6 = GlHyV * GlHyAD
AtAdV7 = GlTpV * GlTpAD
AtAdV8 = LaGlV * LaGlAD
LaGlV = LaGlF + LaGlB + RlAGl
AtAdV9 = PrGlV * PrGlAD
AtAd10 = absGl * abGlAD
AtAd11 = absAa * abAaAD
AtAd12 = kidwrk * EBW * * 0.75
AtAd13 = hrtwrk * Oxup1
AtAd14 = reswrk * Oxup1
AtAd15 = (AaUr + AmUr) * ATAmUr
AtAd16 = (1.0 – effprg) * FMEREQ/AtAdHt
AdAtV = AdAtV1 + AdAtV2 + AdAtV3 + AdAtV4 + AdAtV5
AdAtV1 = GyGlV * GyGlAT
AdAtV2 = TpCdV * TpCdAT
AdAtV3 = PrCdV * PrCdAT
AdAtV4 = BuCdV * BuCdAT
PrCdV = absPr * (1.0 – fPrGl)
BuCdV = absBu
AdAtV5 = GlLa * GlLaAt
'Heat production in viscera'
basHtV = basalV * AtAdHt $ 'basal'
HtV2 = AtAdV3 * AtAdHt $ 'Protein TO'
HtV3 = AtAdV7 * AtAdHt $ 'Gl to Tp'
HtV4 = AtAdV8 * AtAdHt $ 'La to Gl'
HtV5 = AtAd12 * AtAdHt $ 'kidney work'
HtV6 = AtAd13 * AtAdHt $ 'heart work'
HtV7 = AtAd14 * AtAdHt $ 'respiration'
```

```
HIV8 = ATAd15 * AtAdHT $ 'urea synthesis'
MHtV = basHtV + HtV2 + HtV3 + HtV4 + HtV5 + HtV6 + HtV7 + HIV8
```

Oxidative metabolism of glucose, acetate and fatty acids. 'These equations implement the zero pool concept for adenine nucleotides discussed in Chapter 4.'

```
CONSTANT KAcCd = 2.0E – 3,KGlCd = 20.0E – 3,KFaCd = 2.21E – 3
ndAt = AtAd – AdAt
ndOx = ndAt/rtPOx
rtOx1 = cGl * (cAc + KAcCd)/(cAc * (cGl + KGlCd/AHOR))
rtOx2 = cFa * (cAc + KAcCd)/(cAc * (cFa + KFaCd))
GlCd = ((ndOx * rtOx1)/(rtOx1 + rtOx2 + 1.0))/OxGlCd
FaCd = ((ndOx * rtOx2)/(rtOx1 + rtOx2 + 1.0))/OxFaCd
AcCd = (ndOx/(rtOx1 + rtOx2 + 1.0))/OxAcCd
rtPO = (AcCd * AcCdAT + FaCd * FaCdAT + GlCd * GlCdAT)/(AcCd * OxAcCd...
       + FaCd * OxFaCd + GlCd * OxGlCd)
TcHyF = AcTsF * HyAcFa * (1.0 – fGlHyF) $ 'correction for NADPH generated'
TcHyV = AcTmV * HyAcFa * (1.0 – fGlHyV) $ 'by ICD in TCA cycle'
DOx = (LaCdB + LaCdF) * OxLaCd + TpCdV * OxTpCd + PrCdV * OxPrCd + ...
      BuCdV * OxBuCd + AcCd * OxAcCd + FaCd * OxFaCd + GlCd * OxGlCd...
      – TcHyF – TcHyV
```

'Calculation of heat equivalent of ATP. Note that HcLa and HcTp being very close to 1/2 glucose are set exactly to that so energy changes in glycolysis are not represented.'

```
AtHt1 = (LaCdB + LaCdF) * HcLa
AtHt2 = TpCdV * HcTp
AtHt3 = GyGlV1 * (GlGyGY * HcGy – HcGl)
AtHt4 = PrCdV * HcPr
AtHt5 = BuCdV * HcBu
AtHt6 = GlCd * HcGl
AtHt7 = AcCd * HcAc
AtHt8 = FaCd * HcFa
AtHt = AtHt1 + AtHt2 + AtHt3 + AtHt4 + AtHt5 + AtHt6 + AtHt7 + AtHt8
AtAdHt = AtHt/AtAd
```

16.3.7 Summary equations

'Equations that follow are summary equations for specific evaluation purposes. A number of these have been deleted to constrain the length of an already long chapter. Short notes to the effect that such equations are present in the original program have been substituted.'

(a) Milk energy and composition

```
ELm = DMLKLm * 2.0 * HcGl/MWLm
EPm = DMLKPm * HcAa/MWAa
ETm = DMLKTm * HcTg/MWTm
REMLK = ELm + EPm + ETm
PLm = DMLKLm/DMILK
PPm = DMLKPm/DMILK
PTm1 = DMLKTm/DMILK
```


(b) Energy balance and nitrogen retention

'THPI is estimated in the program by summing heat production associated with ea transaction. This is a long section and is not presented here. THPI and THI constitute a cross-check on equations and should be equal within roundoff error.'

```
DBE = DPb * HcAa
DFE = DTsF * HcTg
DVE = DPv * HcAa
EB = DBE + DFE + DVE
THP2 = MEI – EB – REMLK
Nret1 = Nbody + Nmilk
Nabs = (AbsAa * AaFvAm * MWN) + (AbsAm * MWN) $ 'AbsAa and AbsAm in moles'
NUr = Durea * UrAmAm * MWN
Nret2 = Nabs – NUr
Nbody = (DAa + DPb + DPv) * AaFvAm * MWN NMILK = DMLKPm * 0.16
```

(c) Methane emissions

'Methane calculated from model values generated above and by empiric equations.'

```
CH4Efd = CH4E/FDDMIN
fCH4E = CH4E/FDGEin
fCH4DE = CH4E/DEI
fCH4ME = CH4E/MEI
TCH4 = INTEG(DTCH4,ITCH4) $ 'TCH4 is in moles'
CH4KGY = TCH4 * 0.016
CH4MLK = CH4KGY/TVMLK
TCH4E = TCH4 * HCH4
netME = AccMEI/TDMIN
CH4GEI = TCH4E/AccGEI
CH4DEI = TCH4E/AccDEI
```

'Methane calculated (BCH4) using Blaxter and Clapperton (1965) equation.'

```
fFIM = FDDMIN/((100 * EBW * * 0.75)/ME)
mult = MEI/(f1 * 0.110 * EBW * * 0.75)
BCH4 = (1.30 + 0.112 * appDE * 100 + mult * (2.37 – 0.050 * appDE * 100)) * f1
TBCH4 = INTEG(BCH4,1.0E – 8)
```

'Methane calculated according to the equation of Moe and Tyrrell (1979

```
MCH4 = (3.406 + 0.510 * (FDDMIN * (FdSt + FdSc + FdOa + FdPe))...
       + 1.736 * (FDDMIN * FDHc) + 2.648 * (FDDMIN * FDCe)) * f1/4.184
TMCH4 = INTEG(MCH4,1.0E – 8)
```

'A procedural that provides for estimates of income over feed costs under alterr tive milk pricing systems is not presented here.'

'A procedural that calculates energy expenditures associated with each ener transaction in the model and sums these to obtain the estimate of THPI mention above was deleted as was a procedural for estimation of RQ.'

```
END $ 'OF DERIVATIVE'
END $ 'OF DYNAMIC'
END $ 'OF PROGRAM'
```

Evaluations and uses of the model are presented in Chapter 17.

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CHAPTER 17

Evaluation and use of a growth and lactation model

with Lane Ely and K. C. Donovan

There has been a tendency to apply excessively simple economic and applied mathematics to complicated biological problems and, in the process, lose the richness that's implicit in the biology. And, the potential economic gains that are available if the richness is taken into account are lost too.

J. R. Black (personal communication)

17.1 INTRODUCTION

The objectives of this chapter are to illustrate the behavior of the lactating dairy cattle model described in Chapter 16, present sensitivity analyses of effects of varying some key parameter values in the digestion and animal elements and, finally, illustrate the types of data that a dynamic, mechanistic model can generate in support of risk analyses appropriate to evaluations of alternate feeding management strategies as a component of enterprise management.

17.2 BEHAVIORAL ANALYSES

As discussed in previous chapters, behavioral analyses of models are normally undertaken for two reasons. The first is to determine whether or not a model contains provisions adequate to simulation of variance observed in reality. The second is to determine whether or not a model can accurately simulate reality or, as it stands, be used for predictive purposes. Both positive and negative examples will be considered in this section, which illustrate limitations and strengths of the model. Effects of diet and feeding management strategies will be considered in the final section of the chapter. Sensitivity analyses, similarly, can be used for several purposes. One of these is to determine what data are required to estimate parameters not directly measurable using current methods. A related use of sensitivity