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Additional Information

1 **Development of a dynamic model for prediction of energy in milk**  
2 **protein, lactose, fat and enteric methane emissions in goats based on**  
3 **energy balance and indirect calorimetry studies**

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**25 Abstract**

26 Feed costs are overwhelmingly the largest expense for dairy producers. Thus, improving  
27 milk production efficiency (milk fat and protein are the main incomes for farmers) is of  
28 great economic importance in the dairy industry. The main objective of this study was to  
29 develop a dynamic energy partitioning model to describe and quantify how dietary energy  
30 from carbohydrate, protein and fat is transferred to milk (protein, lactose and fat) in dairy  
31 goats. In addition, due to increasing worldwide concerns regarding livestock contribution  
32 to global warming, methane (CH<sub>4</sub>) emission was quantified. For modeling purposes, 158  
33 individual goat observations were used and randomly split into 2/3 for model  
34 development and 1/3 for internal evaluation. For external evaluation, 20 different energy  
35 balance studies from the literature (77 observations) were evaluated. The Root Mean  
36 Square Prediction Error (RMSPE) was 13.2% for loss of energy in CH<sub>4</sub>, 16.8% for energy  
37 in fat, 19.4% for energy in protein and 22.3 energy in lactose. Mean bias was around zero  
38 for all variables and the slope bias was zero for milk energy in lactose, close to 1% for  
39 milk fat (1.01%) and around 3% and 10% for protein and CH<sub>4</sub>, respectively. Random bias  
40 was greater than 85% for energy in CH<sub>4</sub> and milk energy components indicating non-  
41 systematic errors and that the equation in the model fitted the data properly. Analyses of  
42 residuals appeared to be randomly distributed around zero. Slopes of regression lines for  
43 residuals versus predicted were positive for milk fat energy, zero for lactose and negative  
44 for milk energy in protein and CH<sub>4</sub>. This model suggested for use with mixed diets and  
45 by-products to obtain balanced macronutrient supply, methane emissions and milk  
46 performance during mid lactation could be an interesting tool to help farmers simulate  
47 scenarios that increase milk fat and protein, evaluate CH<sub>4</sub> emissions, without the costs of  
48 running animal trials.

49

50 **Lay Summary**

51 The present model using mixed diets with different by-products to obtain macronutrient  
52 balance, methane emission and milk performance during mid lactation could be an  
53 interesting tool to help farmers, without the costs of running animal experiments. The  
54 dietary change from grain-based to partial replacement with agro-industrial-byproducts  
55 in mid-lactation dairy goats was accompanied by transformations in carbohydrate and fat  
56 energy transfer to support production. The output underscored that both oxidation of  
57 carbohydrate and fat interact to maintain milk energy output.

58

59 **Teaser Text**

60 The model allows creating different scenarios with mixed rations and estimating  
61 environmental impact (methane emissions) and the partitioning of milk production into  
62 fat, protein and lactose. Within milk quality, the cheese extract (fat plus protein) is the main  
63 parameter for farmers because the price of milk depends on it.

64

65

66 **Keywords:** dynamic model, energy transfer, mixed diets, lactation, goats

67

68

69 **Abbreviations:** CCC, concordance correlation coefficient; CH<sub>4</sub>, methane; E, energy; HP, heat  
70 production; H<sub>f</sub>, heat of fermentation; HP<sub>x</sub>, heat production from oxidation; OXC, oxidation of  
71 carbohydrate; OXF, oxidation of fat; OXP, oxidation of protein; RE, energy retention; RMSPE,  
72 Root Mean Square Prediction Error

73

## 74 **Introduction**

75 Because feed costs are overwhelmingly the largest expense in dairy farms, higher energy-  
76 related production costs can severely affect livestock producers (Bailey et al., 2005). With  
77 these scaling costs, today more than ever before, producers and nutritionists should focus  
78 on improving feed efficiency without compromising herd health and welfare (Bethard  
79 and Stokes, 1999). In recent years, goat milk production has risen markedly in countries  
80 such as Spain, which produces 22.6% of the goat's milk in the European Union  
81 (FAOSTAT, 2020) ranking second after France (31.9 %). Income over feed cost is a  
82 margin that is calculated as milk revenue per ruminant per day minus feed cost per  
83 ruminant per day. Even though income over feed cost is an ideal tool to measure the  
84 impact of management and feeding decisions, changes in milk component such as fat and  
85 protein are not considered in spite of their large economic impact. In Spain, farmers are  
86 paid based on two components in the milk; protein and fat (protein plus fat is the cheese  
87 extract). Thus, these solids impact milk price and affect the commercial value of milk in  
88 a payment system based on cheese extract (Pirisi et al., 2007).

89 There are growing concerns that ruminants are one of the largest sources of global  
90 methane (CH<sub>4</sub>) emissions. Methane accounts for 14% of total global greenhouse gas  
91 emissions and is 28 times more potent than CO<sub>2</sub> (IPCC, 2014). Enteric CH<sub>4</sub> emissions  
92 from farmed ruminants account for 25% of total CH<sub>4</sub> emissions in the United States (2015  
93 data; US EPA, 2021) and also represent a gross energy loss of 4 to 12% to the ruminant  
94 animal (Johnson and Johnson, 1995). Although most CH<sub>4</sub> emissions come from cattle  
95 (73.8%) and buffalo (11.3%), the remaining 10% comes from small ruminants including  
96 sheep and goats (Gerber, 2013). The world goat population is approximately 1.01 billion  
97 (FAOSTAT, 2020) and produces around 4.61 million tons of enteric CH<sub>4</sub> (around 4.9%  
98 of the total CH<sub>4</sub> emissions from livestock). Likewise, future CH<sub>4</sub> emissions from goats

99 are expected to increase due to enhanced growth of goat populations and demands for  
100 milk and meat.

101 Due to the increase of the feeding costs and concerns about global warming, it is  
102 necessary to pay closer attention to improving nutritional efficiency and milk quality  
103 while controlling or reducing CH<sub>4</sub> emissions. Traditionally, the energy balance of dairy  
104 goats can be estimated by the difference between energy inputs (by feed intake) and the  
105 energy outputs, based on milk yield and body weight of the goats. On commercial farms,  
106 however, calculation of energy balance requires detailed information and facilities that  
107 are not available. These three concerns (nutritional efficiency, milk quality and CH<sub>4</sub>  
108 emissions) could be investigated using modeling tools.

109 The main objective of the present study was to develop a dynamic energy  
110 partitioning model for dairy goats to describe and quantify how the energy from dietary  
111 carbohydrate, protein and fat is transferred to milk (protein, lactose and fat) and the  
112 environment (CH<sub>4</sub> emission).

113

## 114 **Materials and methods**

### 115 *Ethics Statement*

116 The experimental procedures were approved (2021/VSC/PEA/0058) by the Committee  
117 on Animal Use and Care at the Polytechnic University of Valencia (UPV) (Valencia,  
118 Spain), and followed the codes of practice for animals used in experimental work  
119 proposed by the European Union (2003). Authors declare that this manuscript does not  
120 involve ethical issues or affect any endangered or protected species.

### 121 *Experimental data*

122 The core methodology we used was based on a combination of energy and nitrogen  
123 balance with indirect calorimetry. Quantitative measurements of gas exchange in

124 respiration units have been used widely in indirect calorimetry to estimate both heat  
125 production and enteric CH<sub>4</sub> emissions (Chwalibog et al., 1997a; 1997b). In addition, this  
126 methodology allows the estimation of protein, fat and energy retention and mobilization  
127 in the body, oxidation of nutrients and calculation of the energy transfer between protein,  
128 carbohydrate and fat at the whole-body level, as well as the partitioning of energy into  
129 milk protein, lactose and fat.

130 The experiment was conducted at the Experimental Farm from the Institute of  
131 Animal Science and Technology (Universitat Politècnica de Valencia, Spain). Energy and  
132 nitrogen balances were performed in specially designed metabolic cages enabling  
133 individual registration of nutrient intake, milk production and excretion of feces and  
134 urine. The experiment involved 20 multiparous mature Murciano-Granadina dairy goats  
135 in mid-lactation with homogenous body weight (BW;  $47 \pm 4.4$  kg of BW) and milk  
136 production in the previous lactation ( $630 \pm 51$  kg of milk per  $210 \pm 30$  days of lactation).  
137 Two trials with 20 goats per trial in a cross-over design were run with 2 continuous  
138 sampling and gas exchange days (2 samples  $\times$  20 goats  $\times$  2 cross-over  $\times$  2 trials = 160  
139 observations). Goats were fed twice a day with a diet containing 1.0 kg/day of alfalfa and  
140 1.5 kg/day of concentrate; crude protein (CP) ranged between 17-20%, neutral detergent  
141 fiber (NDF) 21-43% and ether extract (EE) 1.8-4%. Energy and nitrogen balance and  
142 real-time gaseous exchange (mobile open-circuit respiration system based on indirect  
143 calorimetry) were measured as described by Fernández et al. (2019). Chemical analyses  
144 were conducted according to methods from AOAC (2012).

145 For modeling purposes, of 160 individual goat samples 2 were removed and 158  
146 individual animal observations were used. Data were randomly split in 2/3 for model  
147 development (106 observations, Table 1) and 1/3 for internal evaluation (52 observations,  
148 Table 2).

149

150 *Model description*

151 The model simulated individual goat milk production and energy partitioning into fat,  
152 protein, lactose, and enteric CH<sub>4</sub> emission at the farm level under an intensive regime  
153 where the animals were fed with mixed rations. The model was conceptually based on  
154 two established models from indirect calorimetry data; the empirical model of Chwalibog  
155 et al. (1997a) was built based on oxidation of nutrients in growing calves and the dynamic  
156 model of energy balance in dairy goats from Fernández (2020).

157 The input of macronutrients (carbohydrates, protein and fat) was measured in  
158 balance experiments, and the outputs included feces, urine and gas emissions. The amount  
159 of retained protein and fat, and the contribution of different substrates to milk fat, protein  
160 and lactose production and the amount of oxidized nutrients were acquired from the  
161 combination of energy balance and gas exchange measurements. All values in the model  
162 and transfer of energy were expressed in energy terms. The calculation of energy  
163 metabolism was carried out with constants and factors accepted in energy metabolism  
164 studies (Brouwer, 1965). The model followed the suggestions by Baumgard et al. (2017)  
165 where the maternal ability is to partition proportionately more of the absorbed nutrients  
166 towards milk synthesis and less into body reserves. The model described below does not  
167 describe intermediary pathways of nutrient metabolism, only the general relationships  
168 between substrates and products.

169 The present model consisted of a dynamic system of differential equations and a  
170 fourth order Runge-Kutta method with an integration step size of 0.05 hour for numerical  
171 integration. The model was run until steady-state was achieved and hour was used as the  
172 unit of time. The model contains fourteen pools (kJ/kg BW<sup>0.75</sup>) represented by the capital  
173 letter Q followed with the name of the pool; (1. Gross energy intake [GEI], 2. Protein



174 intake [PI], 3. Fat intake [FI], 4. Carbohydrate intake [CI], 5. Methane [CH<sub>4</sub>], 6. Ruminal  
 175 volatile fatty acids [VFA], 7. Protein absorbed [PA], 8. Fat absorbed [FA], 9.  
 176 Carbohydrate absorbed [CA], 10. Protein retention [RP], 11. Fat retention [RF], 12. Milk  
 177 protein [MP], 13. Milk lactose [ML], 14. Milk fat [A]). The inputs and outputs to and  
 178 from the pools are the fluxes (kJ/kg BW<sup>0.75</sup> per hour) denoted by the abbreviation F.  
 179 Therefore, the pool changes with time depending on the magnitude of the flux (energy  
 180 transfer among the pools), and the change is described by a differential equation of the  
 181 form:

$$182 \quad \frac{dQ}{dt} = F_{in} - F_{out}$$

183 We developed a model assuming mass action kinetics as follows:

$$184 \quad F_i = k_i \times Q_i$$

185 or

$$186 \quad F_i = k'_i \times Q_i$$

$$187 \quad k'_i = k_i \times \left( \frac{\text{input}}{\text{reference constant}} \right)^n$$

188 Where *i* is the pool name and *n* the exponent. To increase or decrease the speed  
 189 of some fluxes, NDF, EE and metabolizability were used (more details below).

190 Knowledge of the flux and the pool allowed estimation of fractional rate *k*.

$$191 \quad k_i = \frac{F_i}{Q_i}$$

192 Each element of the model is specified by an initial condition derived from actual  
 193 measurements and published literature, and fractional rates are derived mainly from  
 194 experimental and empirical information (energy metabolism calculations). Schematic  
 195 representation of the model is shown in Figure 1 (Stella, 2018). Description of pools and

196 the associated differential equations describing the pool-size change over time are listed  
197 below and abbreviations are referenced in Table 3.

198

199 *1. Gross energy intake pool,  $Q_{\_GEI}$  (kJ/kg  $BW^{0.75}$ ).* This pool includes GEI and has three  
200 outputs. The initial amount of energy intake was determined from DM intake (DMI,  
201 kg/day) multiplied by the energy content of the diet (GE, MJ/kg DM) and divided by the  
202 metabolic BW (kg  $BW^{0.75}$ ), all determined experimentally. Outputs came from splitting  
203 of GEI into protein, fat and carbohydrate fluxes according to dietary protein and fat  
204 content. Fractional rates to protein intake ( $k_{GEI\_PI}$ ), fat intake ( $k_{GEI\_FI}$ ) and carbohydrate  
205 intake ( $k_{GEI\_CI}$ ) were calculated by difference between GEI and PI, FI and CI pools,  
206 respectively. The pools  $Q_{\_PI}$ ,  $Q_{\_FI}$  and  $Q_{\_CI}$  are defined below.

207 *Gross energy intake Pool,  $Q_{\_GEI}$  (kJ/kg  $BW^{0.75}$ ).*

208 Differential equation:

$$209 \quad \frac{dQ_{\_GEI}}{dt} = - F_{GEI\_PI} - F_{GEI\_FI} - F_{GEI\_CI}$$

210 Outputs:

$$211 \quad F_{GEI\_PI} = k_{GEI\_PI} \times Q_{\_GEI}$$

$$212 \quad F_{GEI\_FI} = k_{GEI\_FI} \times Q_{\_GEI}$$

$$213 \quad F_{GEI\_CI} = k_{GEI\_CI} \times Q_{\_GEI}$$

214 The gross energy pool size was expressed by the integral equation:

$$215 \quad GEI = \int_{t_0}^t \frac{dQ_{\_GEI}}{dt} + iGEI$$

216 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
217 ( $t$ ), with  $iGEI$  being the initial pool size (2085 kJ/kg  $BW^{0.75}$  according to Table 1).

218

219 2. Protein intake pool,  $Q_{PI}$  (kJ/kg BW<sup>0.75</sup>). The protein intake pool includes one input  
 220 and two outputs. The amount of protein intake was determined from DMI (kg/day)  
 221 multiplied by the CP content of the diet (g/kg DM) and the heat of combustion of protein  
 222 (Brouwer, 1965):

$$223 \quad PI(kJ) = DMI(kg) \times CP_{diet} \left( \frac{g}{kgDM} \right) \times 23.86 \left( \frac{kJ}{g} \right)$$

224 This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>), all determined  
 225 experimentally (Table 1). The input ( $F_{GEI\_PI}$ ) was defined previously and the two outputs  
 226 were the waste of protein intake from the digestive tract to feces ( $F_{PI\_feces}$ ) and the  
 227 apparent total tract digestibility of protein obtained experimentally (Table 1) and defined  
 228 as  $F_{PI\_PA} = k_{PI\_PA} \times Q_{PI}$ , with fractional rate being  $k_{PI\_PA} = 0.70$  ( $k_{PI\_feces} = 1 - k_{PI\_PA}$ ).

229 Protein energy intake Pool,  $Q_{PI}$  (kJ/kg BW<sup>0.75</sup>).

230 Differential equation:

$$231 \quad \frac{dQ_{PI}}{dt} = F_{GEI\_PI} - F_{PI\_feces} - F_{PI\_PA}$$

232 Input:

$$233 \quad F_{GEI\_PI} = k_{GEI\_PI} \times Q_{GEI}$$

234 Outputs:

$$235 \quad F_{PI\_feces} = k_{PI\_feces} \times Q_{PI}$$

$$236 \quad F_{PI\_PA} = k_{PI\_PA} \times Q_{PI}$$

237 The protein energy intake pool size was expressed by the integral equation:

$$238 \quad PI = \int_{t_0}^t \frac{dQ_{PI}}{dt} + iPI$$

239 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
 240 ( $t$ ), with  $iPI$  being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

241

242 3. Fat intake pool,  $Q_{FI}$  (kJ/kg  $BW^{0.75}$ ). The fat intake pool includes one input and two  
 243 outputs. The amount of fat intake was determined from DMI (kg/day) multiplied by the  
 244 EE content of the diet (g/kg DM) and the fat heat of combustion (Brouwer, 1965):

$$245 \quad FI (kJ) = DMI(kg) \times EE_{diet} \left( \frac{g}{kgDM} \right) \times 39.76 \left( \frac{kJ}{g} \right)$$

246 This expression was divided by the metabolic BW (kg  $BW^{0.75}$ ), all determined  
 247 experimentally (Table 1). The input ( $F_{GEI_{FI}}$ ) was defined above and the two outputs were  
 248 the waste of fat intake from the digestive tract to feces ( $F_{FI_{feces}}$ ) and the apparent total  
 249 tract digestibility of fat obtained experimentally (Table 1) and defined as  $F_{FI_{FA}} = k_{FI_{FA}}$   
 250  $\times Q_{FI}$ , with fractional rate being  $k_{FI_{FA}} = 0.67$  ( $k_{FI_{feces}} = 1 - k_{FI_{FA}}$ ).

251 Fat energy intake Pool,  $Q_{FI}$  (kJ/kg  $BW^{0.75}$ ).

252 Differential equation:

$$253 \quad \frac{dQ_{FI}}{dt} = F_{GEI_{FI}} - F_{FI_{feces}} - F_{FI_{FA}}$$

254 Input:

$$255 \quad F_{GEI_{FI}} = k_{GEI_{FI}} \times Q_{GEI}$$

256 Outputs:

$$257 \quad F_{FI_{feces}} = k_{FI_{feces}} \times Q_{FI}$$

$$258 \quad F_{FI_{FA}} = k_{FI_{FA}} \times Q_{FI}$$

259 The fat energy intake pool size was expressed by the integral equation:

$$260 \quad FI = \int_{t_0}^t \frac{dQ_{FI}}{dt} + iFI$$

261 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
 262 ( $t$ ), with  $iFI$  being the initial pool size (0 kJ/kg  $BW^{0.75}$ ).

263

264 4. Carbohydrate intake pool,  $Q_{CI}$  (kJ/kg BW<sup>0.75</sup>). The carbohydrate intake pool includes  
 265 one input and three outputs. The amount of carbohydrate intake was determined by  
 266 difference as follow:

$$267 \quad CI (kJ) = GEI - PI - FI$$

268 The GEI was obtained experimentally (2085 kJ/kg BW<sup>0.75</sup>, Table 1) and PI and FI  
 269 were defined previously. This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>).  
 270 The input ( $F_{GEI_{CI}}$ ) was defined above and the three outputs were: the excretion of  
 271 carbohydrate intake from the digestive tract to feces ( $F_{CI_{feces}} = k_{CI_{feces}} \times Q_{CI}$ ),  
 272 carbohydrate fermented to VFA ( $F_{CI_{VFA}} = k_{CI_{VFA}} \times Q_{CI}$ ) and carbohydrate that passes  
 273 to the lower intestinal tract ( $F_{CI_{CA}} = k_{CI_{CA}} \times Q_{CI}$ ). The fractional rate  $k_{CI_{feces}}$  was  
 274 defined as 1 minus apparent total tract energy digestibility (1-0.67, Table 1). The  
 275 fractional rate  $k_{CI_{VFA}}$  was obtained according to Demeyer (1992) where it is assumed that  
 276 70% of MEI is supplied as VFA and MEI was obtained experimentally (Table 1). The  
 277 fractional rate  $k_{CI_{CA}}$  was calculated as  $k_{CI_{CA}} = 1 - k_{CI_{feces}} - k_{CI_{VFA}}$ .

278 Carbohydrate energy intake Pool,  $Q_{CI}$  (kJ/kg BW<sup>0.75</sup>).

279 Differential equation:

$$280 \quad \frac{dQ_{CI}}{dt} = F_{GEI_{CI}} - F_{CI_{feces}} - F_{CI_{VFA}} - F_{CI_{CA}}$$

281 Input:

$$282 \quad F_{GEI_{CI}} = k_{GEI_{CI}} \times Q_{GEI}$$

283 Outputs:

$$284 \quad F_{CI_{feces}} = k_{CI_{feces}} \times Q_{CI}$$

$$285 \quad F_{CI_{VFA}} = k_{CI_{VFA}} \times Q_{CI}$$

$$286 \quad F_{CI_{CA}} = k_{CI_{CA}} \times Q_{CI}$$

287

288 The carbohydrate energy intake pool size was expressed by the integral equation:

$$289 \quad CI = \int_{t_0}^t \frac{dQ_{CI}}{dt} + iCI$$

290 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
291 (t), with  $iCI$  being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

292

293 *5. Methane energy waste pool,  $Q_{CH_4}$  (kJ/kg BW<sup>0.75</sup>).* The CH<sub>4</sub> pool had one input,  
294  $F_{VFA_{CH_4}}$ . The CH<sub>4</sub> pool represents the amount of energy losses to the atmosphere from  
295 fermentation in the VFA pool ( $Q_{VFA}$ ). The quantities of CH<sub>4</sub> produced by goats were  
296 obtained experimentally by an open circuit head-hood indirect calorimetry system. Thus,  
297 the fractional rate was calculated as:  $k_{VFA_{CH_4}} = \frac{F_{VFA_{CH_4}}}{Q_{VFA}}$ . The CH<sub>4</sub> flux ( $F_{VFA_{CH_4}}$ ) was  
298 also corrected by NDF and EE of the diet due to the fact that fiber is the main substrate  
299 for methanogens and lipid has an inhibitory effect on ruminal microbial fermentation  
300 (Grainger and Beauchemin, 2011). A reference value of 30% and 3% (average values  
301 from the trial) for NDF and EE, respectively, was used in this model.

302 *CH<sub>4</sub> energy waste Pool,  $Q_{CH_4}$  (kJ/kg BW<sup>0.75</sup>).*

303 Differential equation:

$$304 \quad \frac{dQ_{CH_4}}{dt} = F_{VFA_{CH_4}}$$

305 Input:

$$306 \quad F_{VFA_{CH_4}} = k_{VFA_{CH_4}} \times \left(\frac{NDF}{30}\right)^{0.011} \times \left(\frac{3}{EE}\right)^{0.11} \times Q_{VFA}$$

307 The CH<sub>4</sub> waste energy pool size was expressed by the integral equation:

$$308 \quad CH_4 = \int_{t_0}^t \frac{dQ_{CH_4}}{dt} + iCH_4$$

309 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
310 (t), with  $iCH_4$  being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

311

312 *6.VFA energy pool,  $Q_{VFA}$  (kJ/kg  $BW^{0.75}$ ).* This pool includes one input and three  
 313 outputs. The amount of energy in the VFA was determined according to Demeyer (1992)  
 314 as mentioned above. The input  $F_{Cl_{VFA}}$  and the output  $F_{VFA-CH_4}$  were described earlier.  
 315 The flux  $F_{VFA_{Hf}}$  was the heat of fermentation and was calculated as follows:

316

$$F_{VFA_{Hf}} = HP_{total} - HP_x$$

317

The  $HP_{total}$  was the heat production determined from measurements of  $O_2$   
 318 consumption,  $CO_2$  and  $CH_4$  production, and urine N ( $N_{urine}$ ) using the equation of  
 319 Brouwer (1965):

320

$$HP_{total} \text{ (kJ)} = 16.18 \times O_2 + 5.02 \times CO_2 - 2.17 \times CH_4 - 5.99 \times N_{urine}$$

321

where gases are expressed in liters per day and  $N_{urine}$  in grams per day.

322

The  $CO_2$  production from oxidation ( $CO_{2x}$ ) was calculated as  $CO_2 - (2 \times CH_4)$   
 323 according to Fahey and Berger (1988). Then, HP from oxidation ( $HP_x$ ) was:

324

$$HP_x \text{ (kJ)} = 16.18 \times O_2 + 5.02 \times CO_{2x} - 5.99 \times N_{urine}$$

325

Gases are expressed in liters per day and  $N_{urine}$  in grams per day.

326

$HP_{total}$  and  $HP_x$  were experimentally measured (see Table 1).

327

The flux of VFA to fat absorption pool was calculated as:

328

$$F_{VFA_{FA}} = (Q_{VFA} - F_{VFA_{CH_4}} - F_{VFA_{Hf}}) \times 0.6$$

329

Assuming that 0.6 is the amount of energy from acetic acid that is driving the pool  
 330 of FA according to Ørskov and Ryle (1998) for mixed diets.

331

The amount of energy from VFA that enters the carbohydrate absorption pool was  
 332 obtained by difference.

333

$$F_{VFA_{CA}} = Q_{VFA} - F_{VFA_{CH_4}} - F_{VFA_{Hf}} - F_{VFA_{FA}}$$

334

*VFA energy Pool,  $Q_{VFA}$  (kJ/kg  $BW^{0.75}$ ).*

335

Differential equation:

$$336 \quad \frac{dQ_{VFA}}{dt} = F_{CI_{VFA}} - F_{VFA_{CH4}} - F_{VFA_{Hf}} - F_{VFA_{CA}} - F_{VFA_{FA}}$$

337 Input:

$$338 \quad F_{CI_{VFA}} = k_{CI_{VFA}} \times Q_{CI}$$

339 Outputs:

$$340 \quad F_{VFA_{CH4}} = k_{VFA_{CH4}} \times \left(\frac{NDF}{30}\right)^{0.011} \times \left(\frac{3}{EE}\right)^{0.11} \times Q_{VFA}$$

$$341 \quad F_{VFA_{Hf}} = k_{VFA_{Hf}} \times Q_{VFA}$$

$$342 \quad F_{VFA_{CA}} = k_{VFA_{CA}} \times Q_{VFA}$$

$$343 \quad F_{VFA_{FA}} = k_{VFA_{FA}} \times Q_{VFA}$$

344 The VFA energy pool size was expressed by the integral equation:

$$345 \quad VFA = \int_{t_0}^t \frac{dQ_{VFA}}{dt} + iVFA$$

346 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
347 ( $t$ ), with  $iVFA$  being the initial pool size (0 kJ/kg  $BW^{0.75}$ ).

348

349 *7. Protein absorbed pool,  $Q_{PA}$  (kJ/kg  $BW^{0.75}$ ).* The protein absorbed pool includes two  
350 input and five outputs. The amount of protein absorbed was determined as follow:

$$351 \quad PA (kJ) = PI \left( \frac{kJ}{kg \text{ } BW^{0.75}} \right) \times \left( \frac{CP_{digestibility}}{100} \right)$$

352 It is assumed that the protein pool is equal to the amount of digested protein,  
353 represented by the input  $F_{PI_{PA}}$  that was defined previously, and it could represent the  
354 amount of absorbed amino acids which could be used for milk protein ( $F_{PA_{MP}}$ ), protein  
355 retention ( $F_{PA_{RP}}$ ) or be deaminated ( $F_{RP_{PA}}$ ) and oxidized ( $F_{PA_{OXP}}$ ) with concomitant  
356 excretion of energy with nitrogenous substances in urine ( $F_{PA_{UEN}}$ ) and transferred of  
357 energy to carbohydrate metabolism ( $F_{PA_{CA}}$ ). Feeding systems such as AFRC (1993) and



358 INRA (2018) use metabolizability ( $qm = ME/GE$ ) in the predictions of the efficiency of  
 359 ME use for production. The  $qm$  of the diets was utilized to adjust the flux and a reference  
 360 value of 0.6, obtained from this study, was contemplated (see Tables 1 and 2). The flux  
 361  $F_{PA\_CA}$  was an estimation of gluconeogenesis (generation of glucose from non-carbohydrate  
 362 carbon substrates) and was adjusted by  $qm$ . The fractional rates of  $F_{PA\_RP}$ ,  $F_{PA\_MP}$  and  
 363  $F_{PA\_CA}$  were calculated as  $k = \frac{Flux}{Q_{pool}}$ . See Table 4 for details.

364 The  $F_{PA\_OXP}$  is the energy associated with oxidation of protein and calculated by  
 365 published methods for ruminants (Brouwer, 1958; Chwalibog et al., 1997a);

$$366 \quad F_{PA\_OXP} (kJ) = 6.25 \times N_{urine}(g) \times 18.42 \left( \frac{kJ}{g} \right)$$

367 The fractional rate was calculated from bioenergetic equations and constants. This  
 368 expression was divided by the metabolic BW ( $kg BW^{0.75}$ ). The  $F_{PA\_UEN}$  was the loss of  
 369 energy nitrogen in urine and calculate according to Chwalibog et al. (1997a; 2004):

$$370 \quad F_{PA\_UEN}(kJ) = N_{urine}(g) \times 0.9 \times 24.9 \left( \frac{kJ}{g} \right)$$

371 This expression was divided by the metabolic BW ( $kg BW^{0.75}$ ).

372 *Protein energy Pool,  $Q_{PA}$  ( $kJ/kg BW^{0.75}$ ).*

373 Differential equation:

$$374 \quad \frac{dQ_{PA}}{dt} = F_{PI\_PA} + F_{RP\_PA} - F_{PA\_MP} - F_{PA\_RP} - F_{PA\_OXP} - F_{PA\_UEN} - F_{PA\_CA}$$

375 Input:

$$376 \quad F_{PI\_PA} = k_{PI\_PA} \times Q_{PI}$$

$$377 \quad F_{RP\_PA} = k_{RP\_PA} \times Q_{RP}$$

378 Outputs:

$$379 \quad F_{PA\_MP} = k_{PA\_MP} \times Q_{PA}$$

$$380 \quad F_{PA\_RP} = k_{PA\_RP} \times Q_{PA}$$

$$381 \quad F_{PA\_OXP} = k_{PA\_OXP} \times Q_{PA}$$

$$382 \quad F_{PA\_UEN} = k_{PA\_UEN} \times Q_{PA}$$

$$383 \quad F_{PA\_CA} = k_{PA\_CA} \times \left(\frac{0.6}{qm}\right) \times Q_{PA}$$

384 The protein energy pool size was expressed by the integral equation:

$$385 \quad PA = \int_{t_0}^t \frac{dQ_{PA}}{dt} + iPA$$

386 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
387 ( $t$ ), with  $iPA$  being the initial pool size ( $0 \text{ kJ/kg BW}^{0.75}$ ).

388

389 *8. Fat absorbed pool,  $Q_{FA}$  ( $\text{kJ/kg BW}^{0.75}$ ).* The fat absorbed pool includes four input and  
390 four outputs. The amount of fat absorbed was determined as follows:

$$391 \quad FA (kJ) = FI \left( \frac{kJ}{kg \text{ BW}^{0.75}} \right) \times \left( \frac{EE_{digestibility}}{100} \right)$$

392 It is assumed that the fat pool is equal to the amount of digested fat that was  
393 previously defined by the flux  $F_{FI\_FA}$ . This pool is constituted by the next inputs: digested  
394 fat ( $F_{FI\_FA}$ ), VFA as acetic acid from ruminal fermentation ( $F_{VFA\_FA}$ ), energy transfer from  
395 the carbohydrate pool to FA ( $F_{CA\_FA}$ ), and the mobilization of fat reserves to the fat pool  
396 ( $F_{RF\_FA}$ ). The flux  $F_{CA\_FA}$  was an estimation of lipogenesis (process of producing palmitic  
397 acid and triacylglycerol) and was corrected by  $qm$ ; when diet  $qm$  is high, the  $F_{CA\_FA}$  is  
398 lower and vice versa. The outputs represent the amount of absorbed fatty acids and energy  
399 which could be used for milk fat synthesis ( $F_{FA\_MF}$ ), fat retention ( $F_{FA\_RF}$ ) or mobilization  
400 and oxidation ( $F_{FA\_OXF}$ ) with concomitant excretion of energy-free nitrogen in urine  
401 ( $F_{FA\_UENfree}$ ). Because fiber stimulates milk fat synthesis, provides lipogenic substrates in  
402 the form of acetate and hydroxybutyrate (Van Kneegsel et al., 2007), the flux  $F_{FA\_MF}$  was  
403 corrected by NDF.

404 The  $F_{FA\_OXF}$  is the energy associated with the oxidation of fat and calculated by  
 405 published methods for ruminants (Brouwer, 1958; Chwalibog et al., 1997a);

$$406 \quad F_{FA\_OXF} (kJ) = (1.719 \times O_2 - 1.719 \times CO_{2x} - 1.963 \times N_{urine}) \times 39.76 \left( \frac{kJ}{g} \right)$$

407 This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>). The speed of  
 408 energy transfer from the flux  $F_{FA\_OXF}$  to the environment was adjusted by  $qm$  (being 0.6  
 409 the reference value). The  $F_{FA\_UENfree}$  was the loss of nitrogen energy in urine and  
 410 calculated according to Chwalibog et al. (1997a; 2004):

$$411 \quad F_{FA\_UENfree}(kJ) = UE_{calorimetric\ bomb} (kJ) - F_{PA\_UEN}$$

412 Where  $UE$  was the heat of combustion of urea energy determined in a bomb  
 413 calorimeter. This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>).

414 The fractional rate of the remaining fluxes was calculated as  $k = \frac{Flux}{Q_{pool}}$ . See Table  
 415 3 and 4 for details.

416 *Fat energy Pool,  $Q_{FA}$  (kJ/kg BW<sup>0.75</sup>).*

417 Differential equation:

$$418 \quad \frac{dQ_{FA}}{dt} = F_{FI\_FA} + F_{VFA\_FA} + F_{CA\_FA} + F_{RF\_FA} - F_{FA\_MF} - F_{FA\_RF} - F_{FA\_OXF} - F_{FA\_UENfree}$$

419 Input:

$$420 \quad F_{FI\_FA} = k_{FI\_FA} \times Q_{FI}$$

$$421 \quad F_{VFA\_FA} = k_{VFA\_FA} \times Q_{VFA}$$

$$422 \quad F_{CA\_FA} = k_{CA\_FA} \times \left( \frac{0.6}{qm} \right) \times Q_{CA}$$

$$423 \quad F_{RF\_FA} = k_{RF\_FA} \times Q_{RF}$$

424 Outputs:

$$425 \quad F_{FA_{MF}} = k_{FA_{MF}} \times \left( \frac{NDF}{30} \right)^{0.01} \times Q_{FA}$$

$$426 \quad F_{FA_{RF}} = k_{FA_{RF}} \times Q_{FA}$$

$$427 \quad F_{FA_{OXF}} = k_{FA_{OXF}} \times \left( \frac{0.6}{qm} \right) \times Q_{FA}$$

$$428 \quad F_{FA_{UENfree}} = k_{FA_{UENfree}} \times Q_{FA}$$

429 The fat energy pool size was expressed by the integral equation:

$$430 \quad FA = \int_{t_0}^t \frac{dQ_{FA}}{dt} + iFA$$

431 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
432 ( $t$ ), with  $iFA$  being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

433

434 *9. Carbohydrate absorbed pool,  $Q_{CA}$  (kJ/kg BW<sup>0.75</sup>).* The carbohydrate absorbed pool  
435 includes three inputs and four outputs. The amount of carbohydrate absorbed was  
436 determined as follows:

$$437 \quad CA (kJ) = DE \left( \frac{kJ}{kg BW^{0.75}} \right) - PA - FA$$

438 Where DE is the digestible energy. This carbohydrate pool includes the  
439 contribution of energy from digested carbohydrates ( $F_{CI_{CA}}$ ), from ruminal fermentation  
440 ( $F_{VFA_{CA}}$ ) and gluconeogenesis ( $F_{PA_{CA}}$ ), and it is assumed that under normal feeding  
441 conditions the daily net value of glycogen depots remains constant. The carbohydrate  
442 pool outputs released energy into milk lactose ( $F_{CA_{ML}}$ ), and energy used for lipogenesis  
443 ( $F_{CA_{FA}}$ ), which is evaluated as the amount of energy transferred from carbohydrate to fat  
444 pool. This pool also represent energy-containing products excreted with urine  
445 ( $F_{CA_{UENfree}}$ ) and oxidized carbohydrate ( $F_{CA_{OXC}}$ ).

446 The  $F_{CA\_OXC}$  is the energy associated with oxidation of carbohydrates and  
 447 calculated by published methods for ruminants (Brouwer, 1958; Chwalibog et al., 1997a);

$$448 \quad F_{CA\_OXC} (kJ) = (-2.968 \times O_2 + 4.174 \times CO_{2x} - 2.446 \times N_{urine}) \times 17.85 \left(\frac{kJ}{g}\right)$$

449 This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>). This calculation  
 450 was needed to obtain the fractional rate and the flux was corrected with qm. The  
 451  $F_{CA\_UENfree}$  is the loss of nitrogen energy in urine and calculated according to Chwalibog  
 452 et al. (1997a; 2004):

$$453 \quad F_{CA\_UENfree}(kJ) = UE_{calorimetric\ bomb} (kJ) - F_{PA\_UEN}$$

454 Where UE was the heat of combustion of urea energy determined in a bomb  
 455 calorimeter. This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>).

456 The fractional rate of the remaining fluxes was calculated as  $k = \frac{Flux}{Q_{pool}}$ . See Table  
 457 3 for details.

458 *Carbohydrate energy Pool,  $Q_{CA}$  (kJ/kg BW<sup>0.75</sup>).*

459 Differential equation:

$$460 \quad \frac{dQ_{CA}}{dt} = F_{CI\_CA} + F_{VFA\_CA} + F_{PA\_CA} - F_{CA\_ML} - F_{CA\_FA} - F_{CA\_OXC} - F_{CA\_UENfree}$$

461 Input:

$$462 \quad F_{CI\_CA} = k_{CI\_CA} \times Q_{CI}$$

$$463 \quad F_{VFA\_CA} = k_{VFA\_CA} \times Q_{VFA}$$

$$464 \quad F_{PA\_CA} = k_{PA\_CA} \times \left(\frac{0.6}{qm}\right) \times Q_{PA}$$

465 Outputs:

$$466 \quad F_{CA\_ML} = k_{CA\_ML} \times Q_{CA}$$

$$467 \quad F_{CA\_FA} = k_{CA\_FA} \times \left(\frac{0.6}{qm}\right) \times Q_{CA}$$

$$468 \quad F_{CA\_OXC} = k_{CA\_OXC} \times \left(\frac{qm}{0.6}\right) \times Q_{CA}$$

$$469 \quad F_{CA\_UENfree} = k_{CA\_UENfree} \times Q_{CA}$$

470 The carbohydrate energy pool size was expressed by the integral equation:

$$471 \quad CA = \int_{t_0}^t \frac{dQ_{CA}}{dt} + iCA$$

472 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
473 ( $t$ ), with  $iCA$  being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

474

475 *10. Protein retention pool,  $Q_{RP}$  (kJ/kg BW<sup>0.75</sup>).* The protein-retained pool includes one  
476 input and one output. The amount of protein retained was determined as follows:

$$477 \quad RP (kJ) = N_{retained}(g) \times 6.25 \left(\frac{g \text{ Protein}}{g \text{ of N}}\right) \times 23.86 \left(\frac{kJ}{g \text{ Protein}}\right)$$

478 This expression was divided by the metabolic BW (kg BW<sup>0.75</sup>). The input was  
479  $F_{PA\_RP}$  and the output  $F_{RP\_FA}$ , both defined previously.

480 *Protein retention Pool,  $Q_{RP}$  (kJ/kg BW<sup>0.75</sup>).*

481 Differential equation:

$$482 \quad \frac{dQ_{RP}}{dt} = F_{PA\_RP} - F_{RP\_FA}$$

483 Input:

$$484 \quad F_{PA\_RP} = k_{PA\_RP} \times Q_{PA}$$

485 Outputs:

$$486 \quad F_{RP\_FA} = k_{RP\_FA} \times Q_{RP}$$

487 The protein retention pool size was expressed by the integral equation:

$$488 \quad RP = \int_{t_0}^t \frac{dQ_{RP}}{dt} + iRP$$

489 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
 490 ( $t$ ), with iRP being the initial pool size ( $28 \text{ kJ/kg BW}^{0.75}$ , see Table 1).

491

492 *11. Fat retention pool,  $Q_{RF}$  ( $\text{kJ/kg BW}^{0.75}$ ).* The fat-retained pool includes one input and  
 493 one output. The amount of fat retained was determined as follows:

$$494 \quad RF (kJ) = RE (kJ) - RP (kJ)$$

495 Where RE is the retention of energy and RP the retention of protein (Table 1).

496 This expression was divided by the metabolic BW ( $\text{kg BW}^{0.75}$ ). The input was  $F_{FA\_RF}$  and

497 the output  $F_{RF\_FA}$ , from which energy is retained in body fat or released, respectively. We

498 have observed during the trial that the level of ME of the diet influenced the degree of

499 energy mobilization or deposition in the body (retention of energy negative or positive).

500 As AFRC (1993) and INRA (2018) submitted that tissue gain or mobilization depend of

501  $qm$ , we have corrected as follows: when  $qm > 0.6$  it indicated a positive energy balance

502 in which dietary energy was used for milk production and accumulation of reserve. When

503  $qm < 0.6$  it indicated a negative energy balance and that energy reserves were used for

504 milk production. Thus, fractional rates changed with  $qm$  as follows:

505 if ( $qm \geq 0.6$ )

$$506 \quad \{k_{FA\_RF} = 0.84$$

$$507 \quad k_{RF\_FA} = 0.66$$

508 else

$$509 \quad k_{FA\_RF} = 0.66$$

$$510 \quad k_{RF\_FA} = 0.84\}$$

511

512 The fractional rate constant values used were those proposed by Kebreab et al.  
 513 (2003) for dairy cows, i.e. 0.84 for efficiency of energy gain and 0.66 for efficiency of  
 514 tissue energy mobilization.

515 *Fat retention Pool,  $Q_{RF}$  (kJ/kg  $BW^{0.75}$ ).*

516 Differential equation:

$$517 \quad \frac{dQ_{RF}}{dt} = F_{FA_{RF}} - F_{RF_{FA}}$$

518 Input:

$$519 \quad F_{FA_{RF}} = k_{FA_{RF}} \times Q_{FA}$$

520 Outputs:

$$521 \quad F_{RF_{FA}} = k_{RF_{FA}} \times Q_{RF}$$

522 The fat retention pool size was expressed by the integral equation:

$$523 \quad RF = \int_{t_0}^t \frac{dQ_{RF}}{dt} + iRP$$

524 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
 525 ( $t$ ), with  $iRF$  being the initial pool size (100 kJ/kg  $BW^{0.75}$ , see Table 1).

526

527 *12. Milk protein energy pool,  $Q_{MP}$  (kJ/kg  $BW^{0.75}$ ).* This pool is the energy accumulated  
 528 in the milk protein fraction and had one input,  $F_{PA_{MP}}$ . The energy flux was described as  
 529 a mass action type. MP was the energy content in milk observed from milk protein in the  
 530 trial and it was used as reference to calculate the fractional rate  $k_{PA_{MP}}$ . MP was calculated  
 531 experimentally as follows:

$$532 \quad MP = MY \left( \frac{g}{d} \right) \times Milk\ Protein \left( \frac{g}{100g} \right) \times 23.64 \left( \frac{kJ}{g} \right)$$

533 Where MY was milk production and this expression was divided by the metabolic  
 534 BW (kg  $BW^{0.75}$ ).



535 *Milk protein energy Pool,  $Q_{MP}$  (kJ/kg BW<sup>0.75</sup>).*

536 Differential equation:

$$537 \quad \frac{dQ_{MP}}{dt} = F_{PA_{MP}}$$

538 Input:

$$539 \quad F_{PA_{MP}} = k_{PA_{MP}} \times Q_{PA}$$

540 The MP energy pool size was expressed by the integral equation:

$$541 \quad MP = \int_{t_0}^t \frac{dQ_{MP}}{dt} + iMP$$

542 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
543 (t), with iMP being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

544

545 *13. Milk lactose energy pool,  $Q_{ML}$  (kJ/kg BW<sup>0.75</sup>).* This pool is the energy accumulated  
546 in the milk lactose fraction and had one input,  $F_{CA_{ML}}$ . The energy flux was described as  
547 a mass action type. ML was the energy content in milk observed from milk lactose in the  
548 trial and was used as reference to calculate the fractional rate  $k_{CA_{ML}}$ . ML was calculated  
549 experimentally as follows:

$$550 \quad ML = MY \left( \frac{g}{d} \right) \times \text{Milk Lactose} \left( \frac{g}{100g} \right) \times 17.36 \left( \frac{kJ}{g} \right)$$

551 Where MY was milk production and this expression was divided by the metabolic  
552 BW (kg BW<sup>0.75</sup>).

553 *Milk lactose energy Pool,  $Q_{ML}$  (kJ/kg BW<sup>0.75</sup>).*

554 Differential equation:

$$555 \quad \frac{dQ_{ML}}{dt} = F_{CA_{ML}}$$

556 Input:

$$557 \quad F_{CA\_ML} = k_{CA\_ML} \times Q_{CA}$$

558 The ML energy pool size was expressed by the integral equation:

$$559 \quad ML = \int_{t_0}^t \frac{dQ_{ML}}{dt} + iML$$

560 Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
561 (t), with iML being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

562

563 *14. Milk fat energy pool,  $Q_{MF}$  (kJ/kg BW<sup>0.75</sup>).* This pool is the energy accumulated in the  
564 milk fat fraction and had one input,  $F_{FA\_MF}$ . MF was the energy content in milk observed  
565 from milk fat in the trial and it was used as a reference to calculate the fractional rate  
566  $k_{FA\_MF}$ . MF was calculated experimentally as follows:

$$567 \quad MF = MY \left( \frac{g}{d} \right) \times Milk\ Fat \left( \frac{g}{100g} \right) \times 39.33 \left( \frac{kJ}{g} \right)$$

568 Where MY was milk production and this expression was divided by the metabolic  
569 BW (kg BW<sup>0.75</sup>).

570 *Milk fat energy Pool,  $Q_{ML}$  (kJ/kg BW<sup>0.75</sup>).*

571 Differential equation:

$$572 \quad \frac{dQ_{MF}}{dt} = F_{FA\_MF}$$

573 Input:

$$574 \quad F_{FA\_MF} = k_{FA\_MF} \times \left( \frac{NDF}{30} \right)^{0.01} \times Q_{FA}$$

575

576 The MF energy pool size was expressed by the integral equation:

$$577 \quad MF = \int_{t_0}^t \frac{dQ_{MF}}{dt} + iMF$$

578           Representing the quantity of energy accumulated from initial time ( $t_0$ ) to final time  
579 (t), with iMF being the initial pool size (0 kJ/kg BW<sup>0.75</sup>).

#### 580 *Parameter estimation*

581           The dynamic model used the function *ode()* of the deSolve (solving differential  
582 equations) package for numerical solutions of initial first order problems and was  
583 implemented in R software (2016). The solution was achieved using the lsoda integration  
584 method with absolute and relative error tolerance of  $10^{-6}$ . The parameter estimation was  
585 performed by minimizing the negative log likelihood using the function *optim()* from R  
586 (2016, v.1.1.447) and the method used for optimization was Broyden Fletcher Goldfarb  
587 Shanno algorithm (L-BFGS-B).

588           To characterize model inadequacy (i.e. bias) in the range of our observations, the  
589 observed values of MP, ML, MF and CH<sub>4</sub> emissions were compared with model  
590 predictions and the discrepancy was calculated as the root mean square prediction error  
591 (RMSPE). The RMSPE was decomposed into error due to overall bias of prediction  
592 (mean bias), error due to deviation of the regression slope from unity (slope bias), and  
593 error due to disturbances or random variations (random bias) (Bibby and Toutenburg,  
594 1977). The adequacy of the best-fitting model was further assessed outside the range of  
595 our observations by fitting a regression line between observed and predicted values and  
596 considering the intercept and slope deviation from 0 and 1, respectively. This exercise  
597 extrapolates to zero and beyond the maximum observed values and, thus, quantifies the  
598 applicability domain for the model under consideration.

599           Residual plots [(observed – predicted) versus predicted values] verifying the  
600 assumptions that errors are normally and identically distributed around zero with constant  
601 variance were examined. Since residuals are not correlated with predictions, if the model  
602 is unbiased, the slope of the regression of residuals on predictions must be zero.

603 Furthermore, RMSPE and concordance correlation coefficients (CCC) were also used to  
604 evaluate the precision and accuracy of predicted versus observed values for the model  
605 (Lin, 1989). The CCC estimate represents the product of two components. The first  
606 component is the Pearson correlation coefficient that measures precision (deviation of  
607 observations from the best fit line). The second component is the bias correction factor  
608 that indicates accuracy (i.e. how far the regression line deviates from the unity line).

609

#### 610 *Evaluation of the mathematical model*

611 From the 158 individual animal observations obtained during the experiment, 2/3 were  
612 used to develop the model (106 observations, Table 1) and 1/3 were used for internal  
613 evaluation (52 observations, see Table 2 for details). For external evaluation, the model  
614 was evaluated with data from 20 different energy balance studies from the literature (77  
615 observations, Table 5).

#### 616 *Model internal and external evaluation.*

617 Residual analysis was assessed for adequacy of the model. Comparisons between  
618 observed and model prediction values were performed for MP, ML, MF and CH<sub>4</sub>  
619 emissions. An assessment of the error of the predicted relative to the observed values was  
620 made by calculation of the RMSPE. The prediction error was assessed by calculating the  
621 MSPE. The MSPE was decomposed into mean, slope and random bias, as previously  
622 described. Residual plots verifying the assumptions that errors are normally and  
623 identically distributed around zero with constant variance were examined. The CCC,  
624 described above, evaluates the degree of deviation between the best fit line and the  
625 identity line ( $y=x$ ), thus, the CCC of a model that is closer to 1 is an indicator of better  
626 model performance.

627

## 628 **Results**

### 629 *Model development*

630 The model achieved the steady-state at 24 hours. The model had four parameters and was  
 631 fitted using observations from 106 data. From the input's (body weight, gross energy, qm,  
 632 protein, carbohydrate and fat intake and digestibility), fractional rates and reference  
 633 constants (Table 4), we obtained the outputs: milk energy partition into protein (MP),  
 634 lactose (ML), fat (MF) and CH<sub>4</sub> emissions. Initial and final values of optimized  
 635 parameters, obtained by RMSPE, with their SD and coefficient of variation (CV) are  
 636 shown in Table 4. The parameters  $k_{VFA\_CH_4}$  had a CV of 18% and less than 10% for  
 637 parameters related with milk composition  $k_{PA\_MP}$ ,  $k_{CA\_ML}$ ,  $k_{FA\_MF}$ . The prediction errors  
 638 are shown in Table 6. From lower to higher, the RMSPE were 13.2% for loss of energy  
 639 in CH<sub>4</sub>, 16.8% for MF, 19.4% for MP and 22.3% ML. Evaluation through CCC was in  
 640 agreement with RMSPE, with the largest CCC for milk CH<sub>4</sub> energy (0.643) followed by  
 641 MF (0.574), MP (0.514) and ML (0.464). Mean bias was around zero for all variables and  
 642 the slope bias was zero for energy ML, close to 1% for MF (1.01%) and around 3% and  
 643 10% for MP and CH<sub>4</sub>, respectively. Random bias was greater than 85% for energy in CH<sub>4</sub>  
 644 and milk energy components indicating the absence of non-systematic error, and that the  
 645 equation in the model fitted the data properly.

646 Figure 2 displays observed versus predicted values and the corresponding unity  
 647 regression equation (i.e. observed = predicted). The model had the least bias for MP data  
 648 in the range 80-125 kJ/kg BW<sup>0.75</sup> per day, but below this range it underestimated and  
 649 above this range it overestimated (Figure 2a). For ML, the model bias was minimal  
 650 (Figure 2b). MF also had a nearly unbiased fit to data from 240-280 kJ/kg BW<sup>0.75</sup> per day  
 651 (Figure 2c), and below this range it overestimated and above it underestimated. For  
 652 energy in CH<sub>4</sub> with a narrow range about 80-90 kJ/kg BW<sup>0.75</sup> per day, the model bias was

653 minimal, but below and above this range it underestimated and overestimated,  
654 respectively (Figure 2d). The residual standard error for MP, ML, MF and energy in CH<sub>4</sub>  
655 was off by 23.08, 22.22, 43.84 and 11.36 kJ/kg BW<sup>0.75</sup> per day, respectively.

656 Analyses of residuals are shown in Figure 3. Results are consistent with the biases  
657 illustrated in Figure 2. The ranges shown before residuals appeared to be randomly  
658 distributed about 0. Slopes of regression lines for residuals versus predicted were negative  
659 for MP (Figure 3a) and CH<sub>4</sub> (Figure 3d) indicating that the model overpredicted as the  
660 prediction increased. For ML the slope was 0 (Figure 3b). Slope of regression lines for  
661 residuals versus predicted was positive for the MF pool (Figure 3c) indicating that the  
662 model underpredicted amounts of energy in milk as the prediction increased. Therefore,  
663 extrapolating outside the above ranges may yield increasingly-biased predictions.

664

#### 665 *Internal model evaluation*

666 One third of the data obtained from the study was used for internal evaluation (n = 52  
667 observations). The prediction errors are shown in Table 7. From lower to higher, the  
668 RMSPE were 13.7% for loss of energy in CH<sub>4</sub>, 18.5% for MP, 22.9% for ML and 19.2%  
669 for MF energy. RMSPE greater than 20% indicated that some significant variation of ML  
670 energy still remained to be explained. Evaluation through CCC was in agreement with  
671 RMSPE, with the largest CCC for MP and CH<sub>4</sub> and lowest for ML and MF. Mean bias  
672 was around 0 for ML and MF, 0.19% for MP and 0.39% for CH<sub>4</sub>. The slope bias was  
673 lower for ML and MF (0.84% and 2.54%, respectively) and greater for CH<sub>4</sub> and MP  
674 (5.90% and 10.46%, respectively). A slope bias different from 0 indicated a lack of  
675 precision with the internal validation data set. Therefore, random bias was greater for ML  
676 (99.11%) and MF (97.44%) and lower for CH<sub>4</sub> (93.71%) and MP (89.35%). Random bias  
677 around 89% indicated systematic errors for MP and that mechanisms in the model could

678 be improved. The random bias was higher than 85% indicating the absence of  
679 nonsystematic errors and that the equation in the model fitted the data properly.

680 Figure 4 displays observed versus predicted values and the corresponding unity  
681 regression equation (i.e. observed = predicted). The model had the least bias in a narrow  
682 range and MP was underpredicted (Figure 4a), ML overpredicted (Figure 4b), MF  
683 underpredicted (Figure 4c) and CH<sub>4</sub> underestimated at lower values and overestimated at  
684 higher values (Figure 4d). The residual standard error for MP, ML, MF and energy in  
685 CH<sub>4</sub> was off by 19.83, 22.87, 49.63 and 11.77 kJ/kg BW<sup>0.75</sup> per day, respectively.

686 Analyses of residuals are shown in Figure 5. Results are consistent with the biases  
687 illustrated in Figure 4. Slopes of regression lines for residuals versus predicted were  
688 positive for MP energy pool (Figure 5a) and negative for ML, MF and CH<sub>4</sub> (Figures 5b,  
689 5c and 5d). Thus, we observed underprediction when the amount of milk energy in protein  
690 increased, and overprediction for lactose, fat and CH<sub>4</sub>.

691

#### 692 *External model evaluation*

693 Data from 20 energy balance experiments (n = 77) were used for external evaluation of  
694 the model. Goodness of fit is shown in Table 8. The RMSPE value was higher than 20%  
695 indicating that some variation remained to be explained. Evaluation through CCC was in  
696 agreement with RMSPE as we showed previously. The CCC for CH<sub>4</sub> was not calculated  
697 because some literature experiments did not determine CH<sub>4</sub> emissions. Mean bias  
698 represents the accuracy of the model being around 0 for ML, but greater for others, hence,  
699 some disturbances were detected. The slope bias was around 0 for CH<sub>4</sub> (1.17%), but  
700 different from 0 for milk energy components, meaning lack of precision with the external  
701 data set. Random bias was 98.47% for CH<sub>4</sub> energy, 97.28% for MF energy, 97.11% for  
702 MP and 92.83% for MF. Therefore, random bias was higher than 85% indicating the

703 absence of nonsystematic errors and that the equation in the model fitted the data  
704 appropriately.

705 Plots of observed versus predicted values in milk energy composition and CH<sub>4</sub> are  
706 shown in Figure 6. This figure includes 20 data sets from energy balance experiments  
707 from a literature review. Data points from the same experiment share the same color.  
708 Briefly, Figure 6a shows overestimation in MP at higher values, Figure 6b shows  
709 underestimation in ML at lower values. For MF we observed an overestimation (Figure  
710 6c) at greater values and in CH<sub>4</sub> we observed underprediction for all studies (Figure 6d).

711 Analyses of residuals (regressing residuals against predicted values) are shown in  
712 Figure 7, and for an unbiased model the slope of residuals regressed on prediction must  
713 be 0. The slope was negative for MP, ML, MF and CH<sub>4</sub> (Figure 5a, 5b, 5c and 5d,  
714 respectively), being less accurate for extreme values.

715

## 716 **Discussion**

### 717 *Comparable models*

718 The model was conceptually based on two established models from indirect calorimetry  
719 data as previously was mentioned, Chwalibog et al. (1997a) and Fernández et al. (2020).  
720 The Chwalibog et al. (1997a) model was based on a combination of nitrogen and energy  
721 balance with indirect calorimetry which made possible empirical calculations to estimate  
722 protein, fat, energy retention and mobilization in the body. Besides, total heat production  
723 and net substrate oxidation, and energy transfer between protein, carbohydrate and fat at  
724 the whole-body level were calculated. The model evaluated growth and retention of  
725 energy and dynamic changes over time were not contemplated. Fernández et al. (2020)  
726 developed a dynamic model in lactating goats based on energy balance and indirect  
727 calorimetry, assessed daily variation in CH<sub>4</sub> emissions, milk and loss of heat when daily



728 changes in DMI, lipid and fiber were taking place. However, neither oxidation of nutrients  
729 nor partitioning of energy into milk protein, lactose and fat were considered.

730

### 731 *External simulation*

732 We observed some variation among the 20 published studies that could be due to inherent  
733 differences associated with feeding system, diets, treatments, breed, and/or unique  
734 experimental conditions. Below we first discuss those published experiments with the  
735 poorest goodness of fit.

### 736 *External milk protein simulation*

737 The largest overprediction we observed was for MP (Figure 6a), due mainly to the studies  
738 of Silva et al. (2018), Molina-Alcaide et al. (2010) and Romero-Huelva et al. (2012).  
739 Silva et al., (2018) conducted two experiments with lactating Alpine goats studying the  
740 effects of restricted access to feeders. The diet used was formulated to be relatively high  
741 in quality so as to allow opportunity for a rapid rate of ingestion and acceptable  
742 performance with limited feeder access. Milk yield was determined and chemical  
743 composition was obtained with a MilkoScan 400 analyzer (Foss Electric, Hillerød,  
744 Denmark). Experiment 1 was run in mid to late lactation; the restricted feed access  
745 treatment had neither marked negative nor positive effects on feed intake and  
746 performance measures, reflecting considerable flexibility in feeding behavior. Only the  
747 4-hour feeder access treatment reduced milk yield and the concentrations of milk protein,  
748 which the authors could not explain, thus, this lower milk protein obtained caused  
749 overprediction by the model.

750 The study of Molina-Alcaide et al. (2010) evaluated the effect of partial  
751 replacement of concentrate with two types of feed blocks on ruminal protozoa, nitrogen  
752 and energy balance, microbial N flow to the duodenum and milk performance. Granadina

753 breed goats were hand-milked once a day and milk total solid determined by Kjeldahl for  
754 N (protein was obtained multiplied by 6.38). Romero-Huelva et al. (2012) replaced 35%  
755 of a cereal-based concentrate with feed-blocks containing waste tomato fruit or cucumber  
756 in lactating Granadina goats. Milk chemical analysis was conducted as reported by  
757 Molina-Alcaide et al. (2010). It could be possible that the different methods for measuring  
758 milk protein (Kjeldahl-N vs. MilkoScan FT120) was responsible for the observed model  
759 overprediction.

#### 760 *External milk lactose simulation*

761 The underprediction observed in ML (Figure 6b) was mainly due to the study of Tovar-  
762 Luna et al. (2010b). Tovar-Luna et al. (2010b) studied the effect of stage of lactation and  
763 the level of feed intake in Alpine dairy goats. Energy balance in metabolic cages and  
764 indirect calorimetry were used and milk samples were analyzed for protein, lactose and  
765 fat in a MilkoScan 400 analyzer (Foss Electric, Hillerød, Denmark). Goats were fed ad  
766 libitum, but some after ad libitum consumption were restricted to near ME requirements  
767 for maintenance followed by 4-d of fasting. For other does, fasting was immediately  
768 following the ad libitum consumption. Thus, the underprediction observed was detected  
769 under feed restriction and fasting those likely induced physiological adaptations not  
770 considered in the present model.

#### 771 *External milk fat simulation*

772 Based on visual inspection of MF (Figure 6c), the study of Silva et al. (2018) seems to be  
773 responsible for the overestimation observed. Silva et al. (2018) could not explain the low  
774 milk fat concentrations during the 4-h access to feeders in experiment 1 and during the  
775 2-h access to feeders in experiment 2. The present model overpredicts milk fat, being  
776 greater in experiment 1 than 2, but Silva et al. (2018) reported unexpectedly low values.

#### 777 *External methane simulation*

778 The model underestimates CH<sub>4</sub> emissions mainly in the studies of Molina-Alcaide et al.  
779 (2010), Ibáñez et al. (2016), Romero-Huelva et al. (2017), and Fernández et al. (2021b).  
780 Since Silva et al. (2018) did not report CH<sub>4</sub> this study was not used in the analysis. The  
781 study of Molina-Alcaide et al. (2010) did not conduct indirect calorimetry, thus, no heat  
782 production or oxidation of nutrients and CH<sub>4</sub> were available. The CH<sub>4</sub> production was  
783 estimated from Aguilera et al. (2001) as 10.32% of digestible energy. Therefore, the  
784 values were not comparable with the present model predictions.

785 In the study of Ibáñez et al. (2016) the CH<sub>4</sub> model prediction was lower than  
786 observed for all treatments. Murciano-Granadina goats at mid lactation were fed three  
787 alfalfa hay and concentrate-based mixed diets in which concentrate replaced barley grain  
788 with orange pulp or soy hulls. No differences in CH<sub>4</sub> emissions were observed among  
789 diets for observed and model prediction, but on average the model estimated 45 kJ/kg  
790 BW<sup>0.75</sup> lower emission than observed. The challenge in quantifying CH<sub>4</sub> in vivo is well  
791 known. Thus, the observed differences were likely due to the indirect calorimetry  
792 equipment used or the calibration of the equipment during the studies. Ibáñez et al. (2016)  
793 used the equipment described by Fernández et al. (2015) and the present study used an  
794 improved version of the system described by Fernández et al. (2019).

795 Romero-Huelva et al. (2017) using lactating Granadina goats replaced 47% of the  
796 concentrate (corn, wheat bran, sunflower meal and soy flour) with a mixture of fruit waste  
797 that included tomato, citrus pulp, brewer's grain and yeast. The CH<sub>4</sub> was recorded and a  
798 gas analyzer used (ADG MGA3000, Spurling Works, Herts, UK). The study did not detail  
799 information regarding flowmeter and calibration factors used for measuring the gas  
800 exchange. An underestimation was only found for the control group. In the other groups  
801 (mixture of fruit) a reduction of CH<sub>4</sub> was observed and the model adjusted better. The  
802 presence of plant secondary compounds in by-products may promote less CH<sub>4</sub> production

803 as Romero-Huelva et al. (2017) suggested.

804         Fernández et al. (2021b) studied the CH<sub>4</sub> emissions when forage to concentrate  
805 ratios changed during lactation. Murciano-Granadina goats were fed with mixed diets  
806 based on alfalfa and concentrate. One group was fed with the forage to concentrate ratio  
807 of 35:65 during the whole lactation and the present model predicted successfully the CH<sub>4</sub>  
808 emissions. The other group was fed with a ratio 35:65 in early lactation, 50:50 at mid  
809 lactation and 65:35 in late lactation. The worse estimation by the model was obtained  
810 when the ratio changed from 35:65 to 50:50 and to 65:35 (underestimation of 65 kJ/kg  
811 BW<sup>0.75</sup>, on average). Hence, it seems that the model was useful for most of the studies  
812 tested, but the accuracy diminishes when there was a restriction in access to feed, fasting  
813 and changes in the forage to concentrate ratio. These factors could change tissue energy  
814 accretion, presumably with associated nutrient partitioning, and contribute to changes in  
815 milk composition. Clearly, those management aspects and the ensuing physiological  
816 changes were not contemplated in the present model.

817

#### 818 *Modelling predictions with existing energy balance studies*

819 The 20 studies with indirect calorimetry facilities were conducted across Research  
820 Centers. Since most of these did not calculate macronutrient oxidation nor milk energy  
821 partitioning in fat, protein and lactose, the present data enhanced the value of the data by  
822 making predictions with the model.

823         We evaluated, with the present model, the study of Rapetti et al. (2005) conducted  
824 at Istituto di Zootecnia Generale, Università di Milano (Italy). These authors used indirect  
825 calorimetry and fed lactating Saanen goats with forage and forage-free diets (the qm was  
826 greater than 0.6 for all diets). Using data from the non-forage diet (qm = 0.65), the amount  
827 of energy in MP, ML and MF predicted was 67, 98 and 268 kJ/kg BW<sup>0.75</sup> (total energy of

828 434 kJ/kg BW<sup>0.75</sup> similar to the value observed; 444 kJ/kg BW<sup>0.75</sup>), respectively. Due to  
829 the high qm value, enough ME energy was available from carbohydrate and the retention  
830 of energy was positive; the observed energy retention was 143 kJ/kg BW<sup>0.75</sup> and the  
831 predicted was 255 kJ/kg BW<sup>0.75</sup>. Thus, the model could predict the energy transfer when  
832 positive energy balance was observed as follows. Since the diet was predominantly based  
833 in cereals, the oxidation of carbohydrates was higher than fat oxidation (58 vs 30%), the  
834 accretion of fat retention was positive (107 kJ/kg BW<sup>0.75</sup>) favoring the energy transfer  
835 from the FA to RF pool (body fat deposition). The daily transfer of energy from the CA  
836 to FA pool was of 430 kJ/kg BW<sup>0.75</sup> indicating that carbohydrate that is not oxidized  
837 contributed to fat metabolism, either transferred to milk (lipogenesis and esterification)  
838 or oxidized. The predicted energy lost as CH<sub>4</sub> was 96 kJ/kg BW<sup>0.75</sup>, 16 kJ/kg BW<sup>0.75</sup> lower  
839 than observed.

840 We have evaluated the study of Tovar-Luna et al. (2010a) conducted at the  
841 American Institute for Goat Research, Langston University (USA) using indirect  
842 calorimetry in Alpine dairy goats. Different dietary concentrate levels were used and we  
843 selected groups with higher and lower qm. A group of goats in early lactation fed 20%  
844 concentrate had a qm of 0.53, and the amount of energy transferred to MP, ML and MF  
845 was 92, 74 and 249 kJ/kg BW<sup>0.75</sup>, respectively (observed values were 76, 104 and 157  
846 kJ/kg BW<sup>0.75</sup>, respectively). The model predicted storage of body energy as fat of 151  
847 kJ/kg BW<sup>0.75</sup>, and an energy wasted in CH<sub>4</sub> of 68 kJ/kg BW<sup>0.75</sup> (the observed value was  
848 56 kJ/kg BW<sup>0.75</sup>). The original study did not calculate the oxidation of nutrients and the  
849 present model estimated the oxidation of protein at approximately 17% with the oxidation  
850 of carbohydrate (37%) being lower than the oxidation of fat (46%). That is, greater  
851 oxidation of fat than carbohydrate took place, underscoring that we must evaluate the flux  
852 of energy from carbohydrate to fat and also lipid tissue mobilization.

853 The daily energy transfer from the protein pool to the carbohydrate pool was of  
854 43 kJ/kg BW<sup>0.75</sup> (from PA to CA pool), and the transfer from the carbohydrate to the fat  
855 pool was 474 kJ/kg BW<sup>0.75</sup> (from CA to FA pool). The daily accretion of fat reserves was  
856 -33 kJ/kg BW<sup>0.75</sup>, (difference between  $F_{FA\_RF}$  and  $F_{RF\_FA}$ ) denoting that mobilization of  
857 fat reserves took place in order to support deposition of energy as milk fat. The group of  
858 goats fed 60% of concentrate in mid lactation had a qm of 0.62, and the energy transferred  
859 to MP, ML, MF and CH<sub>4</sub> was 112, 78, 212 and 68 kJ/kg BW<sup>0.75</sup> (close to the observed  
860 values 95, 125, 192 and 85 kJ/kg BW<sup>0.75</sup>, respectively), respectively. Thus, total milk  
861 energy predicted was 402 kJ/kg BW<sup>0.75</sup> and the observed 412 kJ/kg BW<sup>0.75</sup>. Due to the  
862 greater ME available with this diet, higher body fat retention than the diet with qm = 0.53  
863 was observed (242 vs 151 kJ/kg BW<sup>0.75</sup> for qm diets of 0.62 and 0.53 respectively) and  
864 the oxidation of carbohydrate was higher, followed by fat and protein oxidation (46%,  
865 33% and 21%, respectively). The accretion of fat reserves was positive (75 kJ/kg BW<sup>0.75</sup>  
866 and day), indicating accumulation of fat.

867 Although theoretical daily simulation of gluconeogenesis was similar between diets  
868 (44 kJ/kg BW<sup>0.75</sup>), lipogenesis was 52 kJ/kg BW<sup>0.75</sup> greater in the diet with a lower qm.  
869 The diet with 20% of concentrate had 60% of alfalfa hay and 43% of NDF while the 60%  
870 concentrate diet had 20% of alfalfa hay and 31% of NDF. According to Van Kneegsel et  
871 al. (2007), a diet with 20% of concentrate should be considered mainly lipogenic because  
872 of the predominance of forage stimulates ruminal production of acetate and butyrate and  
873 the dietary fat provides fatty acids for uptake by tissues. In contrast, a diet with 60% of  
874 concentrate should be considered a glucogenic diet. Therefore, the group with a lower  
875 qm (20% of concentrate) was lipogenic, had greater oxidation of fat (13% greater), greater  
876 fat mobilization, greater lipogenesis, lower retention of fat reserves (151 kJ/kg BW<sup>0.75</sup> vs  
877 242 kJ/kg BW<sup>0.75</sup>) and 37 kJ/kg BW<sup>0.75</sup> more daily milk energy in the form of fat. In

878 lactating ruminants fed isoenergetic diets, lipogenic nutrients can increase the partitioning  
879 of ME into milk (increasing milk fat yield), and consequently decrease partitioning of  
880 ME into body reserves (Van Knegsel et al., 2007).

881 Another center with indirect calorimetry facilities and studies in dairy goats is the  
882 Estación Experimental de Zaidin (CSIC), Granada (Spain). The study of Marcos et al.  
883 (2020) aimed to reduce feeding costs and diminish the negative environmental impact  
884 associated with agro-industrial by-product disposal by replacing 44% of cereal grains  
885 with a mixture of dried distillers' grains, citrus pulp and olive cake in the concentrate of  
886 lactating Murciano-Granadina goats. The diets were isoproteic and isoenergetic and fat  
887 was added to the diet (from 3 to 5%EE, respectively) to increase the energy content of  
888 the by-product diet. The qm was approximately 0.65 in both diets and the NDF was the  
889 same (21%).

890 No negative effects on CH<sub>4</sub> emission and a greater milk fat and protein content  
891 was detected when the agro-industrial by-products were fed. The model predicted milk  
892 protein, lactose and fat with values of 3.5%, 4.1% and 4.9% for the control diet and the  
893 observed values were similar: 3.2%, 5.2% and 4.6%, respectively with exception of  
894 lactose. The quality composition of milk predicted with the diet with agro-industrial by-  
895 products was 2.9%, 3.7% and 4.6% of protein, lactose and fat, respectively and the  
896 observed values were 3.3%, 5.3% and 4.8%. Thus, values were similar with the exception  
897 of lactose that was greater again. Consequently, the diet with more fibrous by-product  
898 was expected to increase ruminal production of acetate and butyrate and reduce  
899 propionate, precursor of lactose in milk (Van Knegsel et al., 2007), but there was no  
900 difference between diets for lactose (5.2%, on average), although these differences were  
901 detected by the model (4.1% vs 3.7%, for control and by-product diet, respectively).

902 It is possible that the higher value of milk lactose observed was because Marcos

903 et al. (2020) assessed it as the difference between the total solids and the sum of protein,  
904 fat and ash. Regarding milk fat, we expected greater estimated values with the by-product  
905 diet because, according to Van Knegsel et al. (2007), it was a lipogenic diet. However,  
906 the lack of difference in milk fat estimated by the model was likely due to the fact that  
907 diets were isoenergetic and Marcos et al. (2020) reported the same NDF value for both  
908 diets (20.7%) and the present model used NDF to adjust milk fat.

909 The CH<sub>4</sub> predicted and observed, for the control diet, was 22 and 26 g/d,  
910 respectively. The CH<sub>4</sub> predicted and observed with the by-product diet was the same (21  
911 g/d) demonstrating that the model was not able to capture the changes in the diet because  
912 the higher fat was not accompanied by a rise in dietary fiber with the agro-industrial by-  
913 products. The model estimated the oxidation of macronutrients that was not calculated by  
914 Marcos et al. (2020). The oxidation of protein was low (15%, on average) due largely to  
915 the fact that protein is not the main source of energy for mammals and goats acquire more  
916 of the energy from oxidation of carbohydrate and fat. Again, due to greater qm (0.65 in  
917 both diets) and identical GEI and NDF, the oxidation of carbohydrate and fat was the  
918 same between diets; being greater the oxidation of carbohydrates (50%) than fat (35%).  
919 Therefore, this is a scenario where similar transfer of energy among protein, carbohydrate  
920 and fat pools between diets was observed, and enough energy was available to support  
921 milk fat and body fat deposition.

922 The last study considered in this discussion was one that replaced portions of  
923 cereal grain in the concentrate with orange leaves and rice straw in lactating Murciano-  
924 Granadina goats (Fernández et al., 2021a). This study was conducted at the Instituto de  
925 Ciencia y Tecnología Animal en la Universitat Politecnica de Valencia (Spain) that has  
926 indirect calorimetry facilities. Again, as most of the studies with dairy goats, the main  
927 objective was to reduce feeding costs by using horticultural byproducts. In this study the



928 control diet had a  $q_m = 0.61$  and the byproduct diet a  $q_m = 0.54$ . For the  $q_m = 0.61$ , the  
929 predicted milk energy in MP, ML and MF was 119, 100 and 268 kJ/kg  $BW^{0.75}$  (3.8%,  
930 4.4% and 5.2%, respectively) and the observed values were similar 128, 105 and 286  
931 kJ/kg  $BW^{0.75}$  (4.1%, 4.6% and 5.5%). Therefore, the cheese extract for predicted and  
932 observed was close, 9.0% and 9.6%, respectively.

933 The  $CH_4$  predicted (29 g/d) and observed value (30 g/d) was similar. For the lower  
934  $q_m$  (0.54) the predicted milk energy in MP, ML and MF were 122, 98 and 342 kJ/kg  
935  $BW^{0.75}$  (4.3%, 4.8% and 7.3%, respectively) and the observed values were 118, 97 and  
936 303 kJ/kg  $BW^{0.75}$  (4.2%, 4.7% and 6.5%). Therefore, the cheese extract for predicted and  
937 observed was again similar, 11.7% and 10.7%, respectively. The  $CH_4$  predicted (28 g/d)  
938 and the observed value (27 g/d) was almost identical. Consequently, the present model  
939 had a good fit for milk energy partitioning and  $CH_4$  emissions, and could forecast the  
940 changes in diet (reduction of cereal grain and increasing agro-industrial byproducts)  
941 increasing milk fat (2.1 points) and cheese extract (from 9% to 11.7%) and a slight  
942 reduction of  $CH_4$  emissions (1 g/d).

943 With the scenario proposed in the study of Fernández et al. (2021a), the group of  
944 goats fed a diet with  $q_m = 0.61$  had greater oxidation of carbohydrate than fat (47% vs  
945 35%), and in the group with a lower  $q_m$  the oxidation of fat was higher than oxidation of  
946 carbohydrate (46% vs 37%). The model revealed a similar trend as in the study of Tovar-  
947 Luna et al. (2010a) with high and low  $q_m$ ; when the  $q_m$  was high, the energy oxidized  
948 from carbohydrate was higher than from fat oxidation and when the  $q_m$  was low and/or  
949 the proportion of fiber increased, less carbohydrate and more fat was oxidized (Van  
950 Knegsel et al., 2007; Derno et al., 2013).

951 We observed that the daily energy flux from the PA to the CA pool was 48 kJ/kg  
952  $BW^{0.75}$  and 56 kJ/kg  $BW^{0.75}$  (for  $q_m$  high and low respectively). Therefore, when the  $q_m$

953 was lower, more energy from PA was transferred to CA to support energy demands  
954 indicating that PA could drive amino acids to body retention and MP, and the deaminated  
955 amino acids also could be used for other pathways such as gluconeogenesis (Chwalibog  
956 et al. 1997b; 2004). The flux of energy from the CA to the FA pool was  $58 \text{ kJ/kg BW}^{0.75}$   
957 lower for the diet with  $q_m = 0.61$  than the diet with  $q_m = 0.54$ . Thus, when  $q_m$  was lower  
958 a surplus of carbohydrate, which is not oxidized, contributed to fat metabolism being  
959 either oxidized or transferred to milk. The process of producing fat (i.e. triacylglycerol)  
960 encompasses lipogenesis and esterification of the fatty acids produced (e.g. palmitate)  
961 followed by storage in the body or secretion into milk (Chwalibog et al. 2004; Harvatine  
962 et al. 2009). The daily accretion of fat reserves was  $-28 \text{ kJ/kg BW}^{0.75}$  (difference between  
963  $F_{FA\_RF}$  and  $F_{RF\_FA}$ ) highlighting that in the diet with lower  $q_m$  mobilization of fat reserves  
964 took place to support milk fat energy production.

965 The present model confirmed the hypothesis proposed by Van Knegsel et al.  
966 (2007) that energy partitioning between milk and body tissue can be altered by feeding  
967 isocaloric diets that differ in lipogenic and glucogenic nutrient content. When diets were  
968 isoenergetic, the model predicted that goats fed a mainly lipogenic diet (higher in forage  
969 and fat) tended to have higher milk fat compared with feeding the glucogenic diet. When  
970 diets were lower in energy, there was increased body fat mobilization and not always a  
971 higher milk fat output.

972

### 973 *Model application in practice*

974 In the Mediterranean countries goat milk production has traditionally been destined for  
975 cheese manufacture, the physicochemical characteristics and composition of raw milk  
976 being essential for successful development of the dairy goat industry and also for the  
977 marketing of the final products. In Spain, farmers are paid based on two components in

978 the milk, protein and fat (cheese extract). The cheese extract is the main parameter for  
979 farmers because the price of milk depends on it (milk price per cheese extract was  
980 0.0937€; consulted 06/23/22 at Lonja de Albacete, Castilla-La Mancha,  
981 www.oviespana.com). The simulation of the study of Tovar-Luna et al. (2010a) showed  
982 a cheese extract of 6.5% and 7.8% for a high and a low qm (0.62 and 0.53, respectively),  
983 and a milk price of 0.61€/L and 0.73€/L of milk produced, respectively for isoenergetic  
984 diets with 60% or 20% of concentrate. The model evaluation of Fernández et al. (2021a)  
985 showed greater cheese extract for the diet with agro-industrial by products (9.0% and  
986 11.7%), and a price of 0.84€/L and 1.10€/L of milk produced for isoenergetic diets based  
987 on cereals or partial replacement of cereals, respectively.

988

## 989 **Conclusions**

990 The model has provided a dynamic description of energy use, which is a useful  
991 framework to test hypotheses of physiological regulation of energy use by dairy goats. It  
992 allowed to shift the focus towards a more efficient transfer of dietary energy into milk  
993 components. Clearly, this model must be improved to cover greater variations in dietary  
994 concentrate and forages, together with stage of lactation, evaluation of body reserves and  
995 the potential impact of climate change (e.g. heat stress).

996

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## 999 **Conflict of interest statement**

1000 The authors have no conflict of interest to report

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1157 **Figure 1.** Diagrammatic representation of the energy partitioning mathematical model in  
1158 dairy goats (using Stella Architect software). See Table 2 for legend.

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1160 **Figure 2.** Observed versus predicted values of milk energy in protein (a), lactose (b) fat  
1161 (c) and energy in methane (d) used for model development in dairy goats [kJ/kg BW<sup>0.75</sup>  
1162 day; BW<sup>0.75</sup> = MBW]. The regression equations were as follow: milk protein energy  $Y =$   
1163  $28.27 + 0.76X$  (standard error = 13.36 and 0.11 for the intercept and slope respectively;  
1164 residual standard error = 23.08;  $R^2 = 0.30$ ); milk lactose energy  $Y = -2.34 + 1.01X$   
1165 (standard error = 14.88 and 0.15 for the intercept and slope respectively; residual standard  
1166 error = 22.22;  $R^2 = 0.31$ ); milk fat energy  $Y = -41.25 + 1.16X$  (standard error = 33.29 and  
1167 0.12 for the intercept and slope respectively; residual standard error = 43.84;  $R^2 = 0.44$ );  
1168 methane  $Y = 24.08 + 0.75X$  (standard error = 7.52 and 0.08 for the intercept and slope  
1169 respectively; residual standard error = 11.36;  $R^2 = 0.42$ ).

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1171 **Figure 3.** Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in  
1172 methane (d) used for model development in dairy goats [kJ/kg BW<sup>0.75</sup> day; BW<sup>0.75</sup> =  
1173 MBW].

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1176 **Figure 4.** Observed versus predicted values of milk energy in protein (a), lactose (b) fat  
1177 (c) and energy in methane (d) used for model internal evaluation in dairy goats [kJ/kg

1178  $BW^{0.75}$  day;  $BW^{0.75} = MBW$ ]. The regression equations were as follow: milk protein  
 1179 energy  $Y = -7.47 + 1.12X$  (standard error = 17.56 and 0.15 for the intercept and slope  
 1180 respectively; residual standard error = 19.83;  $R^2 = 0.51$ ); milk lactose energy  $Y = 6.59 +$   
 1181  $0.91X$  (standard error = 21.61 and 0.21 for the intercept and slope respectively; residual  
 1182 standard error = 22.87;  $R^2 = 0.26$ ); milk fat energy  $Y = 23.37 + 0.94X$  (standard error =  
 1183 50.70 and 0.19 for the intercept and slope respectively; residual standard error = 49.63;  
 1184  $R^2 = 0.32$ ); methane  $Y = 19.72 + 0.76X$  (standard error = 10.95 and 0.12 for the intercept  
 1185 and slope respectively; residual standard error = 11.77;  $R^2 = 0.43$ ).

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1187 **Figure 5.** Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in  
 1188 methane (d) used for model internal evaluation in dairy goats [kJ/kg  $BW^{0.75}$  day;  $BW^{0.75}$   
 1189 = MBW].

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1192 **Figure 6.** Observed versus predicted values of milk energy in protein (a), lactose (b) fat  
 1193 (c) and energy in methane (d) used for model external evaluation in dairy goats [kJ/kg  
 1194  $BW^{0.75}$  day;  $BW^{0.75} = MBW$ ].

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1197 **Figure 7.** Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in  
 1198 methane (d) used for model external evaluation in dairy goats [kJ/kg  $BW^{0.75}$  day;  $BW^{0.75}$   
 1199 = MBW].

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**Table 1.** Descriptive statistics of variables in the database used to develop the milk energy partitioning model and methane for dairy goats (n = 106 observations)

Lactating Dairy Goat fed Mixed Diet				
Variable <sup>1</sup>	Mean	Min.	Max.	SD
<i>Diet Composition (%DM)</i>				
DM	93.3	93.0	94.0	0.45
CP	18.2	17.1	19.5	0.15
EE	2.7	1.8	3.5	0.85
NDF	31.2	21.0	42.0	8.23
NFC	32.5	31.0	35.0	1.63
GE (MJ/kgDM)	17.2	16.8	17.6	0.21
qm	0.60	0.44	0.71	0.061
<i>Apparent digestibility (%)</i>				
CP	70	67	72	1.9
EE	67	53	76	8.3
Energy	67	54	79	5.2
<i>Energy partitioning (kJ/kg BW<sup>0.75</sup> per day)</i>				
GEI	2085	1496	2781	273.1
Protein intake	520	366	705	70.3
Carbohydrate intake	1439	1049	1894	198.3
Fat intake	127	68	220	40.7
Volatile fatty acids	855	597	1140	119.1
Methane	89	57	114	15.3
DE	1389	1007	1807	178.1
Protein absorbed	365	246	508	53.2

Carbohydrate absorbed	936	610	1275	161.7
Fat absorbed	88	36	168	36.4
MEI	1222	853	1628	170.1
HP	657	515	889	92.6
HPx	637	501	858	87.9
HPf	21	6	81	11.3
OXp	114	32	268	44.3
OXC	301	66	558	135.3
OXF	221	19	530	108.6
Protein retention	28	-498	174	84.7
Fat retention	66	-346	827	171.8
Retained energy	94	-390	529	171.9
Energy in milk protein	116	60	182	28.1
Energy in milk lactose	97	46	174	27.7
Energy in milk fat	258	128	395	79.6
Total energy in milk	471	274	684	91.2
<i>Nitrogen balance (g/day)</i>				
Urinary nitrogen	20	10	35	6.7
Retained nitrogen	3	-3	8	3.6
<i>Goat characteristics</i>				
DMI (g/day)	2146	1597	2503	210.1
Body weight (kg)	47	36	55	4.7
Milk yield (kg/day)	2.3	1.1	2.6	0.52

<sup>1</sup> CP = crude protein; EE = ether extract; GE = gross energy; qm = metabolizability; GEI = gross energy intake; DE = digestible energy; MEI = metabolizable energy intake; HP = heat production; HPx = heat production from oxidation; HPf = heat production from fermentation; OXP = protein oxidation; OXC = carbohydrate oxidation; OXF = fat oxidation; DMI = dry matter intake.

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**Table 2.** Descriptive statistics of variables in the evaluation database used to evaluate the milk energy partitioning model and methane for dairy goats (n = 52 observations)

Lactating Dairy Goat fed Mixed Diet				
Variable <sup>1</sup>	Mean	Min.	Max.	SD
<i>Diet Composition (%DM)</i>				
DM	93.2	93.0	94.0	0.40
CP	18.2	17.0	19.4	0.12
EE	2.6	1.8	4.0	0.91
NDF	30.0	21.0	43.0	8.36
NFC	33.0	31.0	35.2	1.75
GE (MJ/kgDM)	17.3	16.9	17.5	0.19
qm	0.60	0.49	0.70	0.050
<i>Apparent digestibility (%)</i>				
CP	69	66	72	1.9
EE	67	54	75	9.1
Energy	68	59	77	4.9

*Energy partitioning (kJ/kg BW<sup>0.75</sup> per day)*

GEI	2054	1497	2651	263.8
Protein intake	511	367	656	67.8
Carbohydrate intake	1417	1060	1886	193.6
Fat intake	126	68	219	42.6
Volatile fatty acids	855	605	1241	126.1
Methane	86	57	113	15.4
DE	1386	1028	1959	187.2
Protein absorbed	357	246	459	51.3
Carbohydrate absorbed	941	628	1427	170.7
Fat absorbed	87	36	167	38.9
MEI	1222	864	1772	180.2
HP	636	517	892	94.4
HPx	617	503	861	89.7
HPf	19	3	45	9.2
OXp	107	22	227	45.9
OXC	289	59	529	127.9
OXF	221	76	552	93.3
Protein retention	33	-226	148	75.9
Fat retention	103	-299	366	151.4
Retained energy	136	-236	422	158.3
Energy in milk protein	118	65	193	29.2
Energy in milk lactose	98	41	188	29.2
Energy in milk fat	272	72	541	92.8
Total energy in milk	489	237	867	131.6

*Nitrogen balance (g/day)*

Urinary nitrogen	14	13	15	2.9
Retained nitrogen	6	5	7	0.3



*Goat characteristics*

DMI (g/day)	2119	1636	2408	210.0
Body weight (kg)	47	39	55	4.4
Milk yield (kg/day)	2.2	1.0	3.7	0.55

<sup>1</sup> CP = crude protein; EE = ether extract; GE = gross energy; qm = metabolizability; GEI = gross energy intake; DE = digestible energy; MEI = metabolizable energy intake; HP = heat production; HPx = heat production from oxidation; HPf = heat production from fermentation; OXP = protein oxidation; OXC = carbohydrate oxidation; OXF = fat oxidation; DMI = dry matter intake.

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**Table 3.** Pools, fluxes and symbols used in the milk energy partitioning and methane for dairy goat model

Label	Description
Energy pools (kJ/kg BW <sup>0.75</sup> )	
Q_GEI	Energy intake
Q_PI	Protein intake
Q_CI	Carbohydrate intake
Q_FI	Fat intake

Q_VFA	Volatile fatty acids
Q_CH <sub>4</sub>	Methane
Q_PA	Protein assimilation
Q_CA	Carbohydrate assimilation
Q_FA	Fat assimilation
Q_RP	Protein retention
Q_FR	Fat retention
Q_MP	Milk protein
Q_ML	Milk lactose
Q_MF	Milk fat

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Energy fluxes (kJ/kg BW<sup>0.75</sup> per hour)

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F <sub>GEL_PI</sub>	energy intake from diet protein
F <sub>GEL_CI</sub>	energy intake from diet carbohydrate
F <sub>GEL_FI</sub>	energy intake from diet fat
F <sub>PI_feces</sub>	energy lost in feces from protein intake
F <sub>PI_PA</sub>	energy absorbed from protein
F <sub>CI_feces</sub>	energy lost in feces from carbohydrate intake
F <sub>CI_CA</sub>	energy absorbed from carbohydrates
F <sub>CI_VFA</sub>	carbohydrate fermentation to volatile fatty acids
F <sub>FI_feces</sub>	energy lost in feces from fat intake
F <sub>FI_FA</sub>	energy absorbed from fat
F <sub>VFA_CA</sub>	volatile fatty acids to carbohydrate absorbed pool
F <sub>VFA_FA</sub>	volatile fatty acids to fat absorbed pool
F <sub>VFA_CH<sub>4</sub></sub>	methane production
F <sub>VFA_Hf</sub>	heat of fermentation
F <sub>PA_RP</sub>	protein retention
F <sub>PA_MP</sub>	protein in milk
F <sub>PA_UEN</sub>	nitrogen urine energy

$F_{PA\_OXP}$	protein oxidation
$F_{PA\_CA}$	gluconeogenesis
$F_{CA\_ML}$	lactose in milk
$F_{CA\_UENfree}$	urine enegy nitrogen free
$F_{CA\_OXC}$	carbohydrate oxidation
$F_{CA\_FA}$	lipogenesis
$F_{FA\_MF}$	fat in milk
$F_{FA\_RF}$	fat retention
$F_{FA\_UENfree}$	urine energy nitrogen free
$F_{FA\_OXF}$	fat oxidation
$F_{RP\_PA}$	mobilization of protein
$F_{RF\_FA}$	mobilization of fat

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Fractional rates (/hour)

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$k_{GEL\_PI}$	fractional rate of $F_{GEL\_PI}$
$k_{GEL\_CI}$	fractional rate of $F_{GEL\_CI}$
$k_{GEL\_FI}$	fractional rate of $F_{GEL\_FI}$
$k_{PI\_feces}$	fractional rate of $F_{PI\_feces}$
$k_{PI\_PA}$	fractional rate of $F_{PI\_PA}$
$k_{CI\_feces}$	fractional rate of $F_{CI\_feces}$
$k_{CI\_CA}$	fractional rate of $F_{CI\_CA}$
$k_{CI\_VFA}$	fractional rate of $F_{CI\_VFA}$
$k_{FI\_feces}$	fractional rate of $F_{FI\_feces}$
$k_{FI\_FA}$	fractional rate of $F_{FI\_FA}$
$k_{VFA\_HF}$	fractional rate of $F_{VFA\_HF}$
$k_{VFA\_CA}$	fractional rate of $F_{VFA\_CA}$
$k_{VFA\_FA}$	fractional rate of $F_{VFA\_FA}$
$k_{VFA\_CH4}$	fractional rate of $F_{VFA\_CH4}$
$k_{PA\_RP}$	fractional rate of $F_{PA\_RP}$

$k_{PA\_UEN}$	fractional rate of $F_{PA\_UEN}$
$k_{PA\_OXF}$	fractional rate of $F_{PA\_OXF}$
$k_{PA\_CA}$	fractional rate of $F_{PA\_CA}$
$k_{PA\_MP}$	fractional rate of $F_{PA\_MP}$
$k_{CA\_UENfree}$	fractional rate of $F_{CA\_UENfree}$
$k_{CA\_OXC}$	fractional rate of $F_{CA\_OXC}$
$k_{CA\_FA}$	fractional rate of $F_{CA\_FA}$
$k_{CA\_ML}$	fractional rate of $F_{CA\_ML}$
$k_{FA\_UENfree}$	fractional rate of $F_{FA\_UENfree}$
$k_{FA\_OXF}$	fractional rate of $F_{FA\_OXF}$
$k_{FA\_MF}$	fractional rate of $F_{FA\_MF}$
$k_{RP\_PA}$	fractional rate of $F_{RP\_PA}$
$k_{FA\_RF}$	fractional rate of $F_{FA\_RF}$
$k_{RF\_FA}$	fractional rate of $F_{RF\_FA}$
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Reference constants	
<hr/>	
HP	heat production
HPx	heat production form oxidation of nutrients
Hf	heat of fermentation
OXF	oxidation of protein
OXC	oxidation of carbohydrates
OXF	oxidation of fat
<hr/>	
Inputs	
<hr/>	
BW (kg)	body weight
DMI (g/kg DM)	dry matter intake
GE (MJ/kg DM)	Dietary gross energy
CP (%DM)	Dietary crude protein
CPd	Apparent digestibility of protein
EE (%DM)	Dietary fat

EEd	Apparent digestibility of fat
MEI (kJ/kg BW <sup>0.75</sup> per day)	Metabolizable energy intake
qm	metabolisability

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**Table 4.** Initial and final parameter estimation and standard deviation of optimized milk energy partitioning and methane dairy goat model parameters, other parameters and pools

Parameters <sup>1</sup>	Initial Values	Final Values	SD	CV (%)
k <sub>VFA_CH4</sub>	0.142	0.110	0.0226	18
k <sub>PA_MP</sub>	0.575	0.567	0.0057	1
k <sub>CA_ML</sub>	0.073	0.075	0.0014	2
k <sub>FA_MF</sub>	0.034	0.030	0.0028	9
Others Parameters	Fractional rates (/hour)			
k <sub>GEI_PI</sub>	0.25	F <sub>GEI_PI</sub> / Q <sub>GEI</sub>		mass action kinetics
k <sub>GEI_CI</sub>	0.69	F <sub>GEI_CI</sub> / Q <sub>GEI</sub>		mass action kinetics
k <sub>GEI_FI</sub>	0.06	F <sub>GEI_FI</sub> / Q <sub>GEI</sub>		mass action kinetics
k <sub>PI_feces</sub>	0.30	F <sub>PI_feces</sub> / Q <sub>PI</sub>		mass action kinetics
k <sub>PI_PA</sub>	0.70	F <sub>PI_PA</sub> / Q <sub>PI</sub>		mass action kinetics
k <sub>CI_feces</sub>	0.05	F <sub>CI_feces</sub> / Q <sub>CI</sub>		mass action kinetics
k <sub>CI_CA</sub>	0.36	F <sub>CI_CA</sub> / Q <sub>CI</sub>		mass action kinetics
k <sub>CI_VFA</sub>	0.60	F <sub>CI_VFA</sub> / Q <sub>CI</sub>		mass action kinetics



$k_{FI\_feces}$	0.31	$F_{FI\_feces} / Q_{FI}$		mass action kinetics
$k_{FI\_FA}$	0.69	$F_{FI\_FA} / Q_{FI}$		mass action kinetics
$k_{VFA\_Hf}$	0.02	$F_{VFA\_Hf} / Q_{VFA}$		mass action kinetics
$k_{VFA\_CA}$	0.35	$F_{VFA\_CA} / Q_{VFA}$		mass action kinetics
$k_{VFA\_FA}$	0.60	$F_{VFA\_FA} / Q_{VFA}$		mass action kinetics
$k_{PA\_RP}$	0.08	$F_{PA\_RP} / Q_{PA}$		mass action kinetics
$k_{PA\_UEN}$	0.06	$F_{PA\_UEN} / Q_{PA}$		mass action kinetics
$k_{PA\_OXP}$	0.58	$F_{PA\_OXP} / Q_{PA}$		mass action kinetics
$k_{PA\_CA}$	0.23	$F_{PA\_CA} / Q_{PA}$	k computed for a $qm=0.6$	mass action kinetics
$k_{CA\_UENfree}$	0.03	$F_{CA\_UENfree} / Q_{CA}$		mass action kinetics
$k_{CA\_OXC}$	0.03	$F_{CA\_OXC} / Q_{CA}$	k computed for a $qm=0.6$	mass action kinetics
$k_{CA\_FA}$	0.53	$F_{CA\_FA} / Q_{CA}$	k computed for a $qm=0.6$	mass action kinetics
$k_{FA\_UENfree}$	0.03	$F_{FA\_UENfree} / Q_{FA}$		mass action kinetics
$k_{FA\_OXF}$	0.03	$F_{FA\_OXF} / Q_{FA}$	k computed for a $qm=0.6$	mass action kinetics
$k_{FA\_RF}$	0.84	$F_{FA\_RF} / Q_{FA}$		Kebreab et al. (2003)
$k_{RP\_PA}$	0.001	$F_{RP\_PA} / Q_{RP}$		mass action kinetics
$k_{RF\_FA}$	0.66	$F_{RF\_FA} / Q_{RF}$		Kebreab et al. (2003)

Pools (kJ/kg BW <sup>0.75</sup> )	Pools (initial values)	Equations	
Q_GEI	2085	$(DMI \times GE_{diet})/BW^{0.75}$	
Q_PI	0	$[(DMI \times CP)/BW^{0.75}] \times 23.86$	
Q_CI	0	GEI - PI - FI	
Q_FI	0	$[(DMI \times EE)/BW^{0.75}] \times 39.76$	
Q_VFA	0	70% of MEI is supplied as VFA	Demeyer (1992)
Q_CH <sub>4</sub>	0	observed from indirect calorimetry system	
Q_PA	0	CI x CP <sub>digestibility coefficient</sub>	
Q_CA	0	DE <sub>intake</sub> - PA - FA	
Q_FA	0	FI x EE <sub>digestibility coefficient</sub>	
Q_RP	28	$[(N \text{ retained})/BW^{0.75}] \times 6.25 \times 23.86$	
Q_RF	66	RE - RP	
Q_MP	0	$[MY \times CP_{milk} \times 23.64]/BW^{0.75}$	
Q_ML	0	$[MY \times Lactose_{milk} \times 17.36]/BW^{0.75}$	
Q_MF	0	$[MY \times Fat_{milk} \times 39.33]/BW^{0.75}$	
Reference constants			

HP	657	$[16.18 \times O_2 + 5.02 \times CO_2 - 2.17 \times CH_4 - 5.99 \times N_{urine}]/BW^{0.75}$	Brouwer (1965)
HPx	637	$[16.18 \times O_2 + 5.02 \times CO_{2x} - 5.99 \times N_{urine}]/BW^{0.75}$	Brouwer (1965)
Hf	21	HP - HPx	
OXp	114	$6.25 \times N_{urine} \times 18.42$	Brouwer (1958); Chwalibog et al. (1997a)
OXc	301	$[(-2.968 \times O_2 + 4.174 \times CO_{2x} - 2.446 \times N_{urine}) \times 17.85]/BW^{0.75}$	Brouwer (1958); Chwalibog et al. (1997a)
OXf	221	$[(1.719 \times O_2 + 1.719 \times CO_{2x} - 1.963 \times N_{urine}) \times 39.76]/BW^{0.75}$	Brouwer (1958); Chwalibog et al. (1997a)
<hr/> <b>Inputs</b> <hr/>			
BW (kg)	47		observed (development database)
DMI (g/day)	2146		observed (development database)
GE (MJ/kg DM)	17.2		observed (development database)
CP (%DM)	18.2		observed (development database)
CPd (%)	70		observed (development database)
EE (%DM)	2.7		observed (development database)
EEd (%)	67		observed (development database)
MEI (kJ/kg BW <sup>0.75</sup> per day)	1222	MEI = GEI - Efeces - Eurine - E <sub>CH4</sub>	
qm	0.60	MEI/GEI	AFRC (1993); INRA (2018)

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<sup>1</sup> Parameters abbreviation is given in Table 2.

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**Table 5.** Summary of the data used for model external evaluation (n = 77 average goats observations)

Lactating Dairy Goat fed Mixed Diet					
Variable <sup>1</sup> (kJ/kg BW <sup>0.75</sup> per day)	Mean	Min.	Max.	SD	
Rapetti et al. (2005)					
<i>Diet Composition (%DM)</i>					
CP (%)	17.6	16.6	18.7	1.05	
NDF (%)	32.0	30.2	34.2	2.04	
EE (%)	2.3	1.8	2.9	0.55	
GE (MJ/kgDM)	18.5	18.3	18.6	0.15	
qm	0.62	0.60	0.65	0.027	
<i>Apparent digestibility (%)</i>					
CP	68	64	72	4.1	
EE	78	72	83	5.3	
<i>Energy partitioning</i>					
GEI	1916	1877	1940	33.5	
Energy in methane	106	97	112	7.8	
MEI	1186	1140	1261	65.7	
Energy in milk	430	424	436	5.6	
Energy in milk protein	127	112	143	15.3	
Energy in milk lactose	126	115	138	11.8	
Energy in milk fat	208	190	232	21.2	
<i>Goat characteristics</i>					
DMI (g/day)	2170	2054	2354	161.4	

Body weight (kg)	53.9	53	55.4	1.27
Milk yield (kg/day)	3.3	3	3.7	0.35
Tovar-Luna et al. (2010a)				
<i>Diet Composition (%DM)</i>				
CP (%)	19.0	17.5	20.4	1.59
NDF (%)	37.2	31.3	43.1	6.46
EE (%)	-	-	-	-
GE (MJ/kgDM)	-	-	-	-
qm	0.55	0.45	0.62	0.068
<i>Apparent digestibility (%)</i>				
CP	68	61	74	5
EE	-	-	-	-
<i>Energy partitioning</i>				
GEI	1638	1486	1731	83.4
Energy in methane	69	50	91	16.3
MEI	905	753	1073	109.5
Energy in milk	316	171	407	86.9
Energy in milk protein	76	45	95	18.3
Energy in milk lactose	96	47	125	28.5
Energy in milk fat	156	86	203	44.2
<i>Goat characteristics</i>				
DMI (g/day)	1660	1460	1740	104.9
Body weight (kg)	51.9	49.1	54.1	1.93
Milk yield (kg/day)	2.3	1.2	2.9	0.65
Tovar-Luna et al. (2010b)				
<i>Diet Composition (%DM)</i>				
CP (%)	18.3	18.3	18.3	0.00
NDF (%)	33.4	33.4	33.4	0.00

EE (%)	-	-	-	-
GE (MJ/kgDM)	-	-	-	-
qm	0.65	0.59	0.69	0.039
<i>Apparent digestibility (%)</i>				
CP	75	70	79	3.8
EE	-	-	-	-
<i>Energy partitioning</i>				
GEI	1330	797	2025	588.2
Energy in methane	54	14	105	29.0
MEI	845	540	1231	326.9
Energy in milk	295	164	485	122.3
Energy in milk protein	71	41	112	27.8
Energy in milk lactose	86	32	162	49.7
Energy in milk fat	144	84	219	56.5
<i>Goat characteristics</i>				
DMI (g/day)	1338	770	1980	576.7
Body weight (kg)	49.8	44.9	55.2	4.05
Milk yield (kg/day)	2.0	0.8	3.6	1.06
Molina-Alcaide et al. (2010)				
<i>Diet Composition (%DM)</i>				
CP (%)	13.2	10.4	15.9	2.75
NDF (%)	16.9	12.7	21.4	4.35
EE (%)	0.3	0.3	0.4	0.07
GE (MJ/kgDM)	14.2	12.5	16.7	2.23
qm	0.58	0.57	0.59	0.012
<i>Apparent digestibility (%)</i>				
CP	71	69	72	1.4
EE	74	70	80	5.3

*Energy partitioning*

GEI	1467	1370	1520	83.9
Energy in methane	104	95	111	8.2
MEI	848	781	899	60.5
Energy in milk	232	218	258	22.8
Energy in milk protein	57	46	75	15.8
Energy in milk lactose	62	49	87	21.7
Energy in milk fat	133	110	175	36.0

*Goat characteristics*

DMI (g/day)	1358	1295	1405	56.6
Body weight (kg)	38.9	38.3	39.5	0.6
Milk yield (kg/day)	1.1	1.0	1.3	0.15

Romero-Huelva et al. (2012)

*Diet Composition (%DM)*

CP (%)	15.9	14.9	17.0	1.01
NDF (%)	44.1	33.8	48.3	6.92
EE (%)	1.2	0.3	3.4	1.49
GE (MJ/kgDM)	16.4	15.6	18.2	1.23
qm	0.61	0.61	0.62	0.005

*Apparent digestibility (%)*

CP	77	76	78	1.0
EE	76	73	80	3.1

*Energy partitioning*

GEI	1823	1770	1930	72.7
Energy in methane	82	67	110	19.3
MEI	1115	1090	1180	43.6
Energy in milk	239	229	251	9.9
Energy in milk protein	54	49	62	5.7



Energy in milk lactose	63	49	80	13.1
Energy in milk fat	143	130	166	16.3
<i>Goat characteristics</i>				
DMI (g/day)	1572	1548	1631	39.5
Body weight (kg)	37	30.2	40.3	4.57
Milk yield (kg/day)	1.0	0.9	1.0	0.04

López and Fernández (2013)

*Diet Composition (%DM)*

CP (%)	18.7	18.6	18.8	0.14
NDF (%)	41.1	34.8	47.5	8.93
EE (%)	3.6	2.1	5.0	2.06
GE (MJ/kgDM)	19.1	18.8	19.4	0.45
qm	0.61	0.60	0.63	0.021

*Apparent digestibility (%)*

CP	70	69	71	1.0
EE	75	66	84	12.4

*Energy partitioning*

GEI	2356	2286	2427	100
Energy in methane	99	96	101	3.5
MEI	1444	1436	1453	11.7
Energy in milk	537	532	542	7.5
Energy in milk protein	124	121	127	4.5
Energy in milk lactose	106	103	110	4.9
Energy in milk fat	316	285	347	43.6

*Goat characteristics*

DMI (g/day)	2070	2040	2100	42.4
Body weight (kg)	43.1	43.1	43.1	0.01
Milk yield (kg/day)	2.2	2.1	2.2	0.09

Ibáñez et al. (2014)

*Diet Composition (%DM)*

CP (%)	15.2	14.7	15.7	0.71
NDF (%)	33.2	30.7	35.7	3.54
EE (%)	2.3	1.9	2.7	0.57
GE (MJ/kgDM)	17.5	17.4	17.5	0.07
qm	0.68	0.65	0.71	0.036

*Apparent digestibility (%)*

CP	76	76	77	0.6
EE	70	60	80	14.6

*Energy partitioning*

GEI	1734	1595	1872	195.9
Energy in methane	77	61	92	21.9
MEI	1182	1044	1320	195.2
Energy in milk	285	277	292	10.6
Energy in milk protein	72	70	75	3.8
Energy in milk lactose	60	59	62	2.1
Energy in milk fat	139	125	152	19.6

*Goat characteristics*

DMI (g/day)	1760	1630	1890	183.8
Body weight (kg)	47	46.8	47.1	0.21
Milk yield (kg/day)	1.3	1.3	1.4	0.04

López et al. (2014)

*Diet Composition (%DM)*

CP (%)	15.8	14.8	16.7	0.66
NDF (%)	39.7	30.1	59.0	16.67
EE (%)	2.3	2.0	2.7	0.24
GE (MJ/kgDM)	17.6	17.2	18.0	0.28

qm	0.69	0.65	0.72	0.026
<i>Apparent digestibility (%)</i>				
CP	70	65	75	3.6
EE	72	70	75	2.5
<i>Energy partitioning</i>				
GEI	1649	1629	1668	18.4
Energy in methane	107	84	118	14.0
MEI	1139	1079	1193	46.5
Energy in milk	400	364	445	37.7
Energy in milk protein	93	89	97	3.6
Energy in milk lactose	83	71	93	9.4
Energy in milk fat	238	206	274	32.7
<i>Goat characteristics</i>				
DMI (g/day)	1535	1508	1570	25.2
Body weight (kg)	41.7	41.4	42	0.22
Milk yield (kg/day)	1.7	1.5	1.9	0.19
Ibáñez et al. (2015)				
<i>Diet Composition (%DM)</i>				
CP (%)	18.1	18	18.2	0.14
NDF (%)	43.6	40.6	46.5	4.17
EE (%)	4.8	4.3	5.3	0.71
GE (MJ/kgDM)	19.1	19.0	19.2	0.14
qm	0.61	0.61	0.62	0.008
<i>Apparent digestibility (%)</i>				
CP	77	76	78	1.4
EE	85	84	86	1.4
<i>Energy partitioning</i>				
GEI	2328	2286	2370	58.9

Energy in methane	95	95	95	0.0
MEI	1423	1411	1435	16.8
Energy in milk	536	530	542	8.4
Energy in milk protein	126	121	132	7.8
Energy in milk lactose	112	107	117	6.9
Energy in milk fat	319	309	330	14.6
<i>Goat characteristics</i>				
DMI (g/day)	2050	2030	2070	28.3
Body weight (kg)	43	43	43	0.0
Milk yield (kg/day)	2,3	2.2	2.4	0.14
Criscioni et al. (2016)				
<i>Diet Composition (%DM)</i>				
CP (%)	16.1	15.8	16.4	0.42
NDF (%)	33.6	31.8	35.3	2.47
EE (%)	1.7	1.6	1.8	0.14
GE (MJ/kgDM)	17	17	17	0.0
qm	0.66	0.63	0.69	0.036
<i>Apparent digestibility (%)</i>				
CP	71	69	74	3.4
EE	61	58	65	4.7
<i>Energy partitioning</i>				
GEI	1650	1591	1709	83.4
Energy in methane	87	82	91	6.4
MEI	1089	1085	1092	4.9
Energy in milk	359	341	376	24.7
Energy in milk protein	100	98	102	2.5
Energy in milk lactose	79	77	82	3.3
Energy in milk fat	189	178	201	15.9

*Goat characteristics*

DMI (g/day)	1700	1600	1800	141.4
Body weight (kg)	45.8	45.6	45.9	0.21
Milk yield (kg/day)	1.7	1.7	1.8	0.08

Criscioni and Fernández (2016)

*Diet Composition (%DM)*

CP (%)	15.7	15.3	16.1	0.57
NDF (%)	25	22.8	27.2	3.11
EE (%)	7.9	4.1	11.7	5.37
GE (MJ/kgDM)	18.7	17.9	19.4	1.06
qm	0.68	0.66	0.71	0.034

*Apparent digestibility (%)*

CP	72	71	73	0.9
EE	74	67	80	8.9

*Energy partitioning*

GEI	1833	1777	1889	79.2
Energy in methane	84	73	95	15.6
MEI	1254	1248	1259	7.8
Energy in milk	508	491	524	23.3
Energy in milk protein	119	117	121	2.4
Energy in milk lactose	104	99	108	7.0
Energy in milk fat	297	266	328	44

*Goat characteristics*

DMI (g/day)	1720	1610	1830	155.6
Body weight (kg)	46.1	45.8	46.4	0.42
Milk yield (kg/day)	2.2	2.1	2.2	0.07

Ibáñez et al. (2016)

*Diet Composition (%DM)*

CP (%)	13.2	11.9	14.0	0.80
NDF (%)	42.5	31.4	54.6	8.23
EE (%)	2.7	1.1	4.8	1.34
GE (MJ/kgDM)	17.8	16.9	18.0	0.48
qm	0.62	0.58	0.65	0.027
<i>Apparent digestibility (%)</i>				
CP	61	56	66	3,5
EE	61	34	74	16
<i>Energy partitioning</i>				
GEI	2174	2056	2296	87.9
Energy in methane	138	130	146	6.1
MEI	1352	1311	1412	47.2
Energy in milk	516	475	572	37.3
Energy in milk protein	116	106	130	8.9
Energy in milk lactose	104	93	115	8.6
Energy in milk fat	308	289	333	19.4
<i>Goat characteristics</i>				
DMI (g/day)	2020	2000	2100	44.7
Body weight (kg)	42.1	41.6	42.4	0.31
Milk yield (kg/day)	2.2	1.9	2.4	0.19

Romero-Huelva et al. (2017)

*Diet Composition (%DM)*

CP (%)	17.7	17.4	18.0	0.42
NDF (%)	28.4	26.9	29.9	2.12
EE (%)	3.3	3.1	3.6	0.31
GE (MJ/kgDM)	16.6	15.8	17.3	1.06
qm	0.67	0.65	0.68	0.026

*Apparent digestibility (%)*

CP	80	79.0	81.0	1.3
EE	-	-	-	-
<i>Energy partitioning</i>				
GEI	1440	1360	1520	113.1
Energy in methane	105	86	123	26.2
MEI	957	930	984	38.2
Energy in milk	-	-	-	-
Energy in milk protein	83	82	83	0.8
Energy in milk lactose	77	73	81	5.1
Energy in milk fat	202	195	210	10.3
<i>Goat characteristics</i>				
DMI (g/day)	1525	1512	1537	17.7
Body weight (kg)	44.5	43.3	45.7	1.70
Milk yield (kg/day)	1.3	1.3	1.3	0.02
Silva et al. (2018)				
<i>Diet Composition (%DM)</i>				
CP (%)	16.6	16.6	16.6	0.0
NDF (%)	40.6	40.6	40.6	0.0
EE (%)	-	-	-	-
GE (MJ/kgDM)	20.6	20.6	20.6	0.0
qm	0.58	0.53	0.65	0.033
<i>Apparent digestibility (%)</i>				
CP	81	79	83	1.8
EE	-	-	-	-
<i>Energy partitioning</i>				
GEI	2109	1906	2662	191.6
Energy in methane	-	-	-	-
MEI	1210	1054	1417	75.9

Energy in milk	300	194	446	80.9
Energy in milk protein	71	48	96	15.8
Energy in milk lactose	83	53	116	23.1
Energy in milk fat	160	99	251	46.1
<i>Goat characteristics</i>				
DMI (g/day)	2111	1874	2695	218.6
Body weight (kg)	56.5	54.3	59.9	1.79
Milk yield (kg/day)	2.3	1.6	3.2	0.62
Fernández et al. (2018)				
<i>Diet Composition (%DM)</i>				
CP (%)	16.5	16.0	17.0	0.71
NDF (%)	26	21	31	7.1
EE (%)	2.5	2.0	3.0	0.71
GE (MJ/kgDM)	16.5	16.0	17.0	0.71
qm	0.6	0.6	0.7	0.046
<i>Apparent digestibility (%)</i>				
CP	70	66	73	5.0
EE	70	68	73	3.3
<i>Energy partitioning</i>				
GEI	1588	1462	1713	177.5
Energy in methane	55	47	63	11.3
MEI	998	970	1025	38.9
Energy in milk	347	336	358	15.6
Energy in milk protein	99	93	106	9.0
Energy in milk lactose	83	83	84	0.7
Energy in milk fat	203	198	209	7.4
<i>Goat characteristics</i>				
DMI (g/day)	1600	1500	1700	141.4



Body weight (kg)	44.1	41.5	46.7	3.68
Milk yield (kg/day)	1.3	0.8	1.7	0.64
Fernández et al. (2019)				
<i>Diet Composition (%DM)</i>				
CP (%)	16.0	14.7	17.3	1.84
NDF (%)	29.0	26.2	31.5	3.70
EE (%)	2.2	2.0	2.3	0.21
GE (MJ/kgDM)	16.5	16.0	17.0	0.71
qm	0.65	0.58	0.72	0.092
<i>Apparent digestibility (%)</i>				
CP	69	67	72	4.0
EE	63	57	70	9.6
<i>Energy partitioning</i>				
GEI	1477	1334	1620	202.2
Energy in methane	50	41	59	12.7
MEI	951	947	954	4.9
Energy in milk	291	281	301	14.1
Energy in milk protein	74	74	75	1.0
Energy in milk lactose	62	62	62	0.4
Energy in milk fat	167	159	175	10.9
<i>Goat characteristics</i>				
DMI (g/day)	1525	1360	1690	233.3
Body weight (kg)	43.3	42.5	44.1	1.13
Milk yield (kg/day)	1.29	1.25	1.33	0.06
Marcos et al. (2020)				
<i>Diet Composition (%DM)</i>				
CP (%)	16.7	16.0	17.4	0.99
NDF (%)	20.7	20.5	20.8	0.21

EE (%)	3.8	2.8	4.7	1.33
GE (MJ/kgDM)				
qm	0.65	0.65	0.66	0.008
<i>Apparent digestibility (%)</i>				
CP	61	46	75	20.7
EE				
<i>Energy partitioning</i>				
GEI	1730	1730	1730	0.0
Energy in methane	76	67	85	12.7
MEI	1130	1120	1140	14.1
Energy in milk	411	393	428	24.7
Energy in milk protein	90	85	94	5.9
Energy in milk lactose	107	103	111	5.7
Energy in milk fat	216	205	227	15.6
<i>Goat characteristics</i>				
DMI (g/day)	1614	1591	1637	32.5
Body weight (kg)	45.3	44.8	45.8	0.71
Milk yield (kg/day)	2.0	2.0	2.1	0.11
Romero et al. (2020)				
<i>Diet Composition (%DM)</i>				
CP (%)	18	18	18	0.0
NDF (%)	38	34	42	5.6
EE (%)	3	2	4	1.4
GE (MJ/kgDM)	16.5	16.0	17.0	0.71
qm	0.59	0.56	0.62	0.037
<i>Apparent digestibility (%)</i>				
CP	69	67	72	3.1
EE	65	53	76	16.3

*Energy partitioning*

GEI	1926	1913	1939	18.38
Energy in methane	85	75	95	14.1
MEI	1138	1095	1180	60.1
Energy in milk	423	402	444	29.7
Energy in milk protein	122	116	128	8.8
Energy in milk lactose	100	97	103	4.3
Energy in milk fat	300	270	330	42.0

*Goat characteristics*

DMI (g/day)	2020	2000	2040	28.3
Body weight (kg)	47.4	47.3	47.4	0.07
Milk yield (kg/day)	2.3	2.2	2.4	0.11

Fernández et al. (2021a)

*Diet Composition (%DM)*

CP (%)	18	18	18	0.0
NDF (%)	38.5	35.0	42.0	4.95
EE (%)	2.3	1.8	2.8	0.71
GE (MJ/kgDM)	16.5	16.0	17.0	0.71
qm	0.57	0.54	0.61	0.056

*Apparent digestibility (%)*

CP	71	70	72	1.2
EE	69	67	71	4.1

*Energy partitioning*

GEI	2203	2189	2217	19.8
Energy in methane	92	88	96	5.7
MEI	1266	1187	1345	111.7
Energy in milk	461	446	476	21.2
Energy in milk protein	123	118	128	7.2

Energy in milk lactose	101	97	105	6.1
Energy in milk fat	294	286	303	12.4
<i>Goat characteristics</i>				
DMI (g/day)	2230	2200	2260	42.4
Body weight (kg)	45.4	45.0	45.7	0.49
Milk yield (kg/day)	2.2	2.1	2.3	0.18
Fernández et al. (2021b)				
<i>Diet Composition (%DM)</i>				
CP (%)	16	16	16	0.0
NDF (%)	32.5	30.0	40.0	4.18
EE (%)	2	2	2	0.0
GE (MJ/kgDM)	16.8	16.0	17.0	0.41
qm	0.59	0.52	0.65	0.055
<i>Apparent digestibility (%)</i>				
CP	69	66	72	2.2
EE	52	42	61	6.9
<i>Energy partitioning</i>				
GEI	1671	1216	1906	259.3
Energy in methane	110	90	126	11.9
MEI	994	629	1196	215.9
Energy in milk	376	222	485	98.7
Energy in milk protein	107	78	150	29.2
Energy in milk lactose	98	67	146	34.3
Energy in milk fat	223	155	326	76.1
<i>Goat characteristics</i>				
DMI (g/day)	1683	1280	1860	219.1
Body weight (kg)	44.6	42.3	47.3	2.04
Milk yield (kg/day)	2.0	1.5	3.0	0.67

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<sup>1</sup> CP = crude protein; EE = ether extract; GE = gross energy; qm = metabolizability; GEI = gross energy intake; MEI = metabolizable energy intake; DMI = dry matter intake.

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**Table 6.** Milk energy partitioning dairy goat model using performance data from the developmental dataset (n=106): prediction errors and decomposition associated with prediction of the outputs (kJ/kg BW<sup>0.75</sup> per day)

Variable	Observed mean	Predicted mean	RMSPE <sup>1</sup> , %	Mean bias, %	Slope bias, %	Random bias, %	CCC <sup>2</sup>
Milk protein energy	116	115	19.4	0.15	3.11	96.75	0.514
Milk lactose energy	97	97	22.3	0.57	0.00	99.43	0.464
Milk fat energy	258	257	16.8	0.00	1.01	98.99	0.574
Methane energy	89	88	13.2	0.01	9.6	90.39	0.643

<sup>1</sup> RMSPE = root mean square prediction error as a percentage of observed mean.

<sup>2</sup> CCC = Concordance Correlation Coefficient.

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**Table 7.** Milk energy partitioning dairy goat model using performance data from the evaluation dataset (n=52): prediction errors and decomposition associated with prediction of outputs (kJ/kg BW<sup>0.75</sup> per day)

Variable	Observed mean	Predicted mean	RMSPE <sup>1</sup> , %	Mean bias, %	Slope bias, %	Random bias, %	CCC <sup>2</sup>
Milk protein energy	118	113	18.5	0.19	10.46	89.35	0.623
Milk lactose energy	98	96	22.9	0.05	0.84	99.11	0.464
Milk fat energy	271	259	19.2	0.02	2.54	97.44	0.489
Methane energy	86	87	13.7	0.39	5.90	93.71	0.646

<sup>1</sup> RMSPE = root mean square prediction error as a percentage of observed mean.

<sup>2</sup> CCC = Concordance Correlation Coefficient.

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**Table 8.** Milk energy partitioning in dairy goat model using literature data from the external evaluation (n=77): prediction errors and decomposition associated with prediction of outputs (kJ/kg BW<sup>0.75</sup> per day)

Variable	Observed mean	Predicted mean	RMSPE <sup>1</sup> , %	Mean bias, %	Slope bias, %	Random bias, %	CCC <sup>2</sup>
Milk protein energy	88	100	26.50	0.41	2.48	97.11	0.425
Milk lactose energy	89	88	26.51	0.02	2.70	97.28	0.430
Milk fat energy	201	194	30.44	0.12	7.05	92.83	0.345

Methane energy	90	92	35.04	0.36	1.17	98.47	-
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<sup>1</sup> RMSPE = root mean square prediction error as a percentage of observed mean.

<sup>2</sup> CCC = Concordance Correlation Coefficient.

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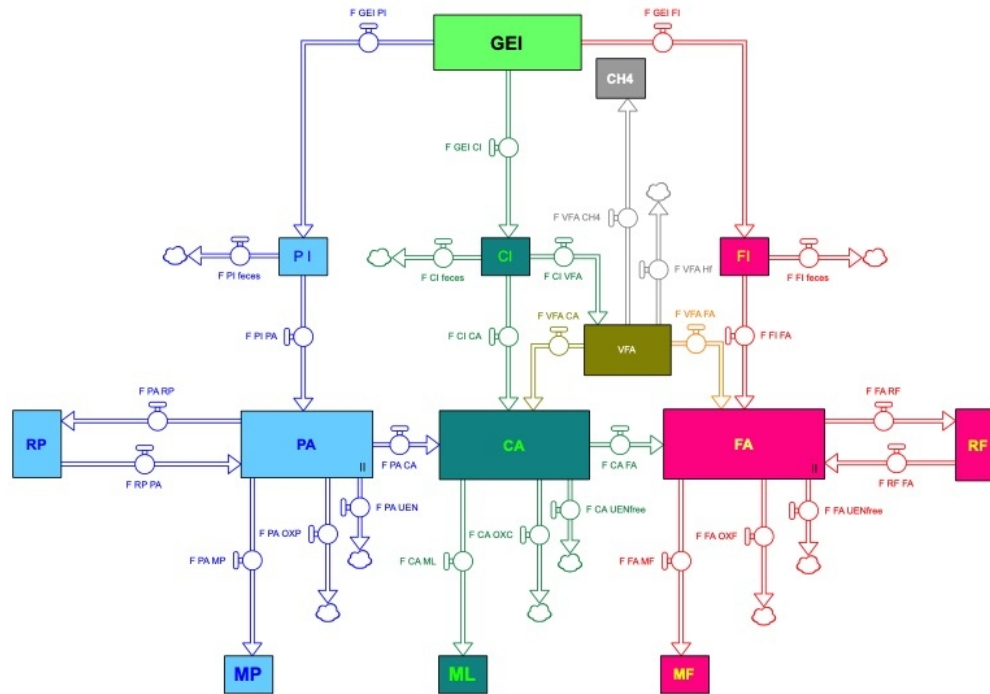


Figure 1. Diagrammatic representation of the energy partitioning mathematical model in dairy goats (using Stella Architect software). See Table 2 for legend.

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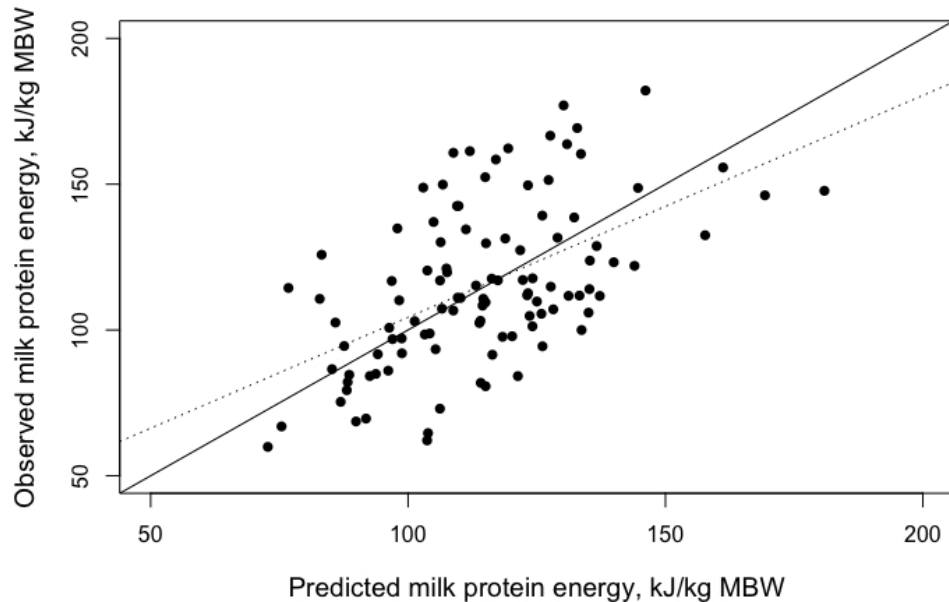
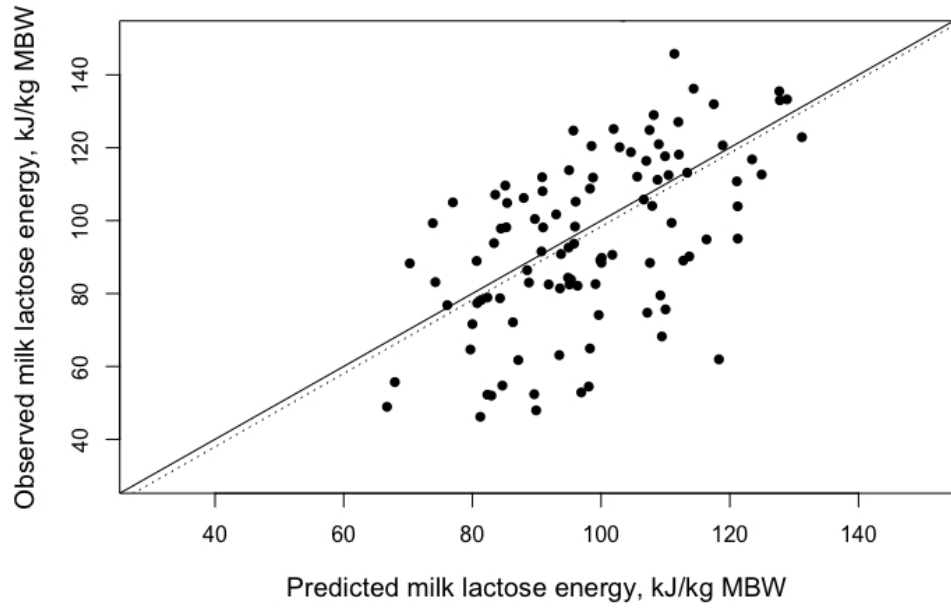
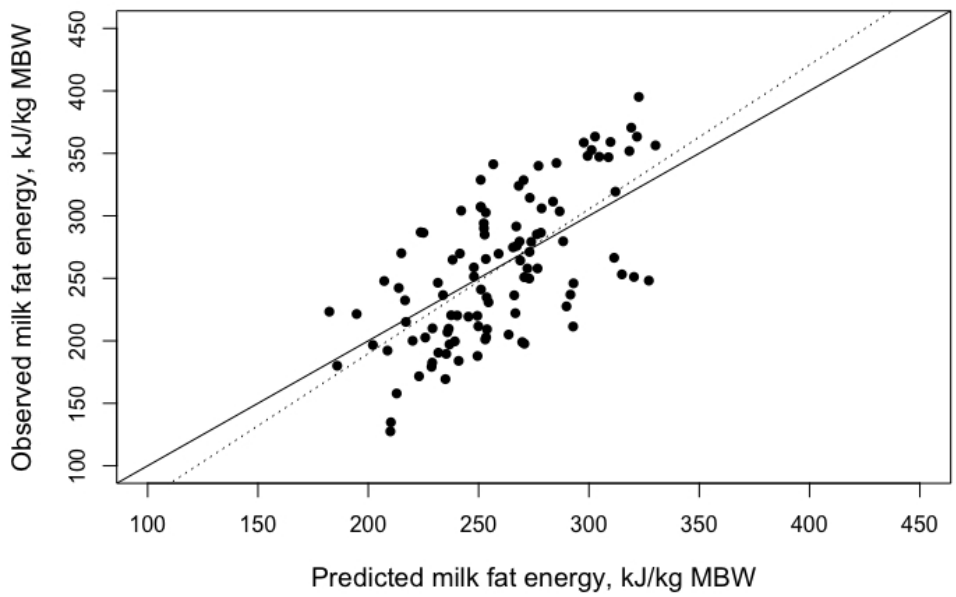


Figure 2. Observed versus predicted values of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model development in dairy goats [kJ/kg BW<sup>0.75</sup> day; BW<sup>0.75</sup> = MBW]. The regression equations were as follow: milk protein energy  $Y = 28.27 + 0.76X$  (standard error = 13.36 and 0.11 for the intercept and slope respectively; residual standard error = 23.08;  $R^2 = 0.30$ ); milk lactose energy  $Y = -2.34 + 1.01X$  (standard error = 14.88 and 0.15 for the intercept and slope respectively; residual standard error = 22.22;  $R^2 = 0.31$ ); milk fat energy  $Y = -41.25 + 1.16X$  (standard error = 33.29 and 0.12 for the intercept and slope respectively; residual standard error = 43.84;  $R^2 = 0.44$ ); methane  $Y = 24.08 + 0.75X$  (standard error = 7.52 and 0.08 for the intercept and slope respectively; residual standard error = 11.36;  $R^2 = 0.42$ ).

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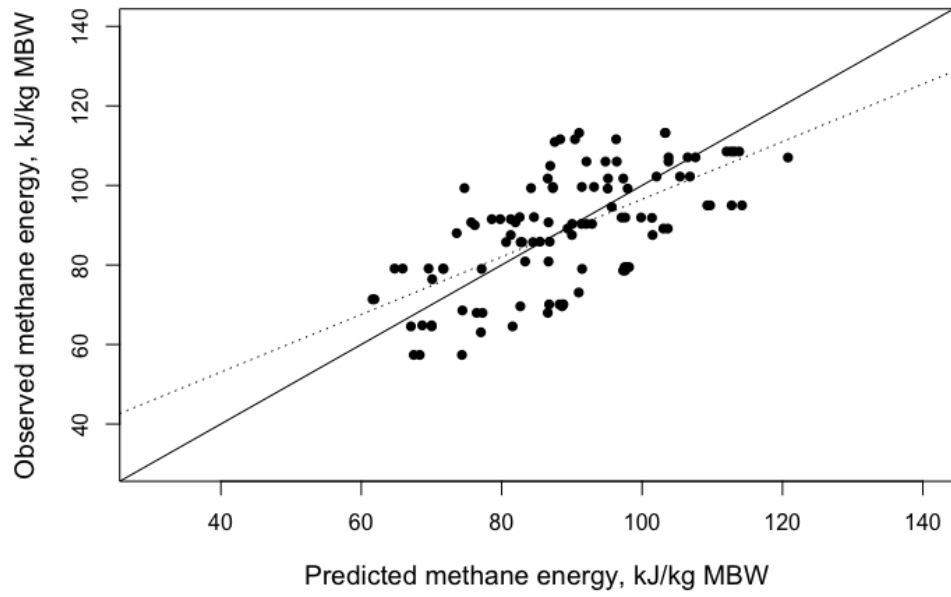


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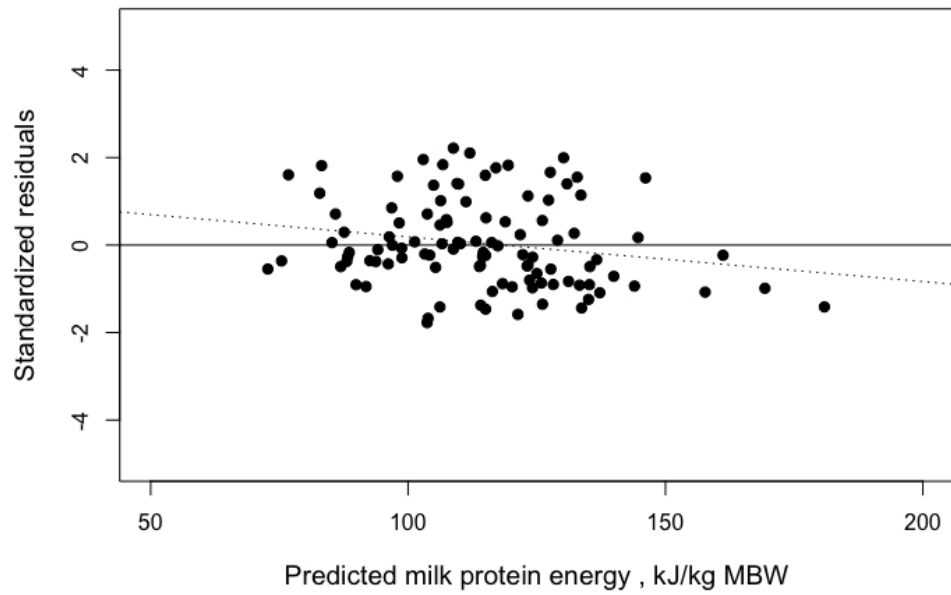
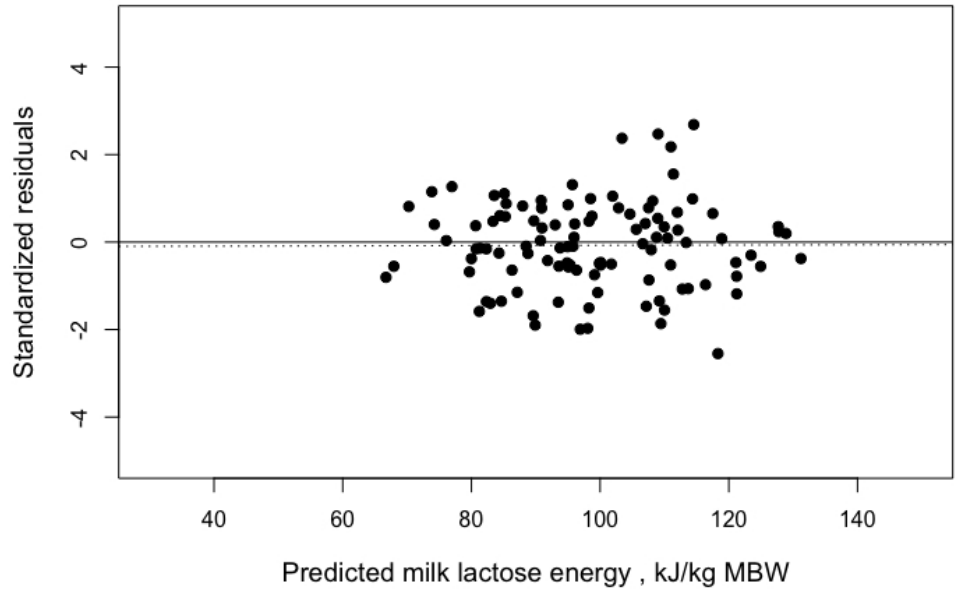
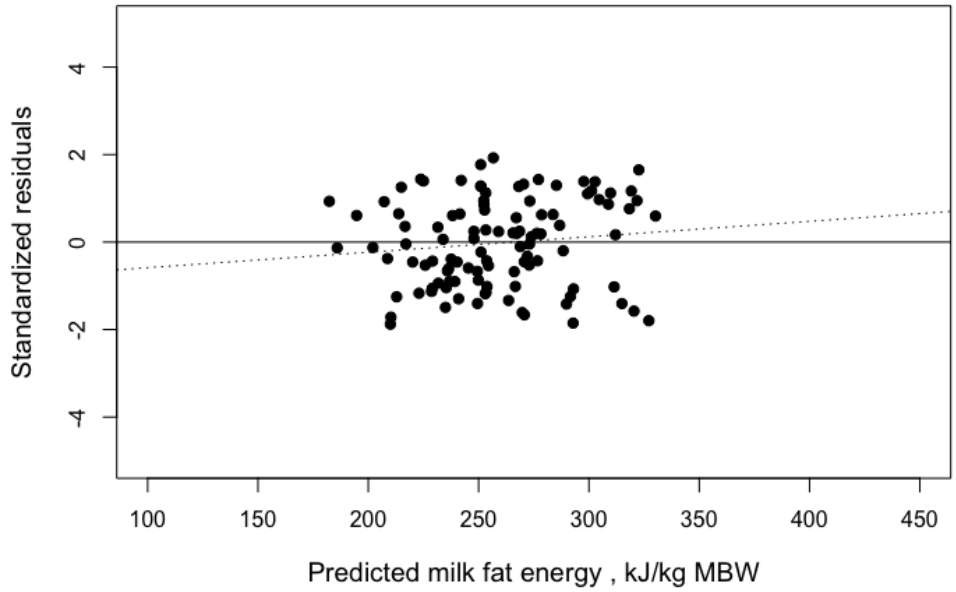


Figure 3. Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model development in dairy goats [kJ/kg BW<sup>0.75</sup> day; BW<sup>0.75</sup> = MBW].

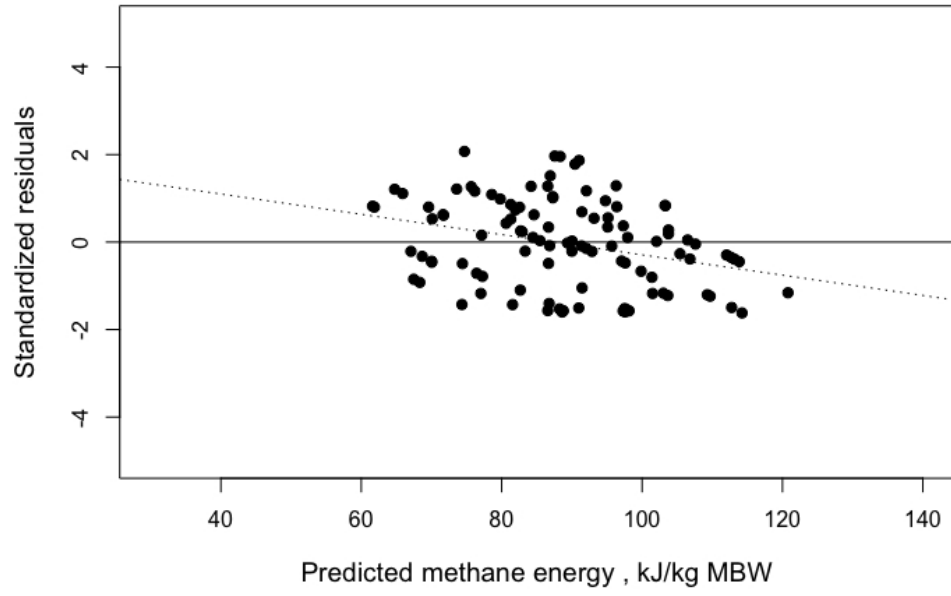
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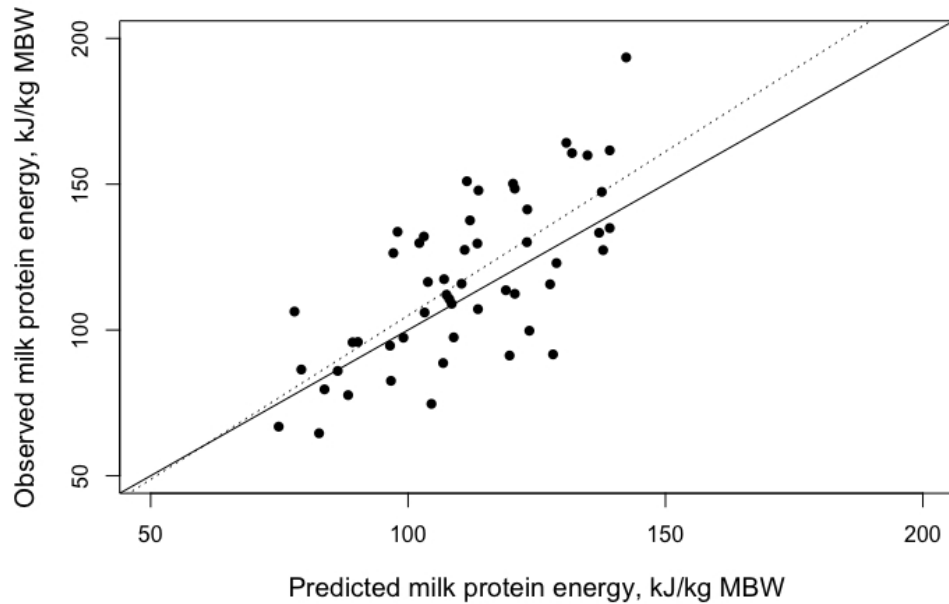
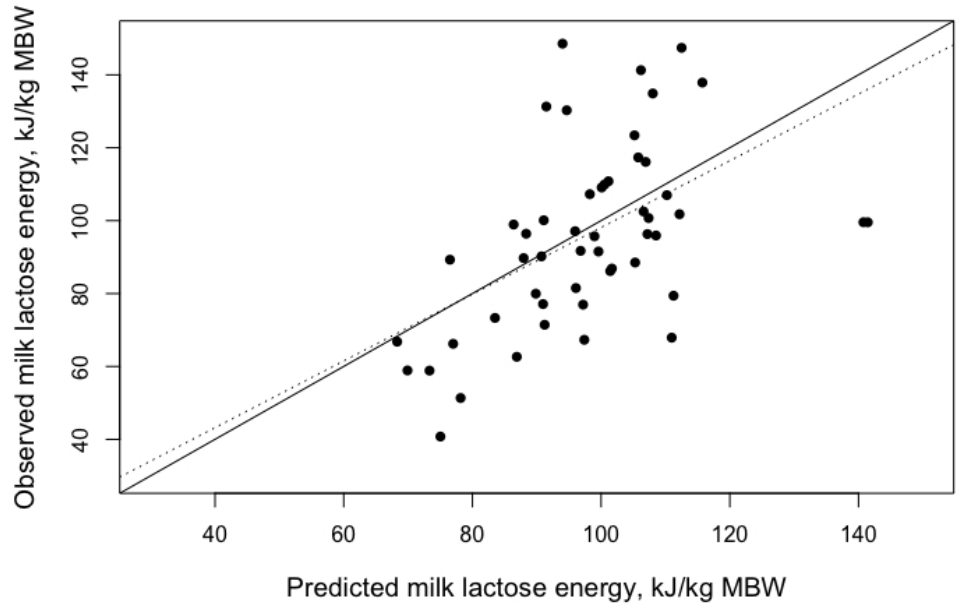
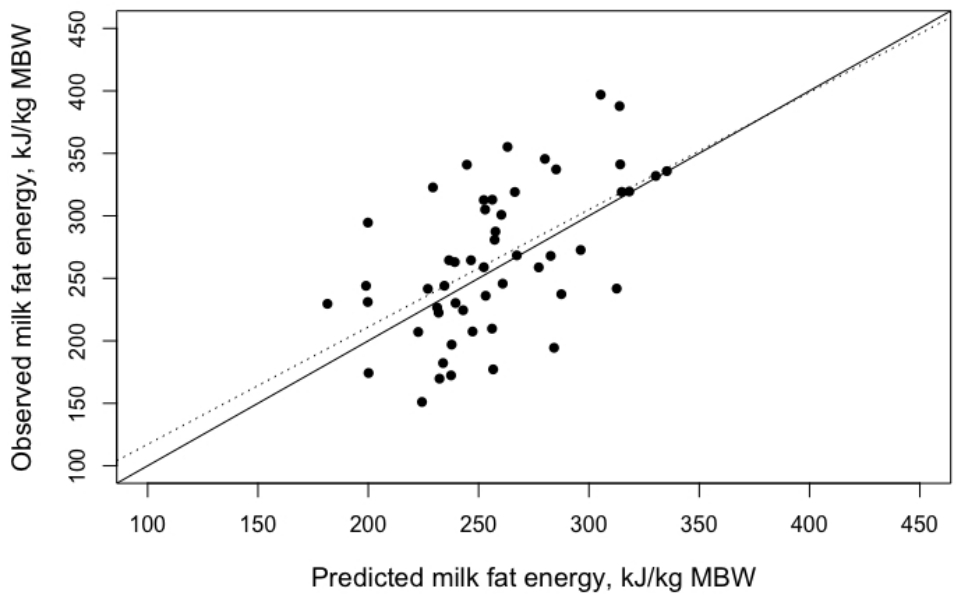


Figure 4. Observed versus predicted values of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model internal evaluation in dairy goats [kJ/kg BW<sup>0.75</sup> day; BW<sup>0.75</sup> = MBW]. The regression equations were as follow: milk protein energy  $Y = -7.47 + 1.12X$  (standard error = 17.56 and 0.15 for the intercept and slope respectively; residual standard error = 19.83;  $R^2 = 0.51$ ); milk lactose energy  $Y = 6.59 + 0.91X$  (standard error = 21.61 and 0.21 for the intercept and slope respectively; residual standard error = 22.87;  $R^2 = 0.26$ ); milk fat energy  $Y = 23.37 + 0.94X$  (standard error = 50.70 and 0.19 for the intercept and slope respectively; residual standard error = 49.63;  $R^2 = 0.32$ ); methane  $Y = 19.72 + 0.76X$  (standard error = 10.95 and 0.12 for the intercept and slope respectively; residual standard error = 11.77;  $R^2 = 0.43$ ).

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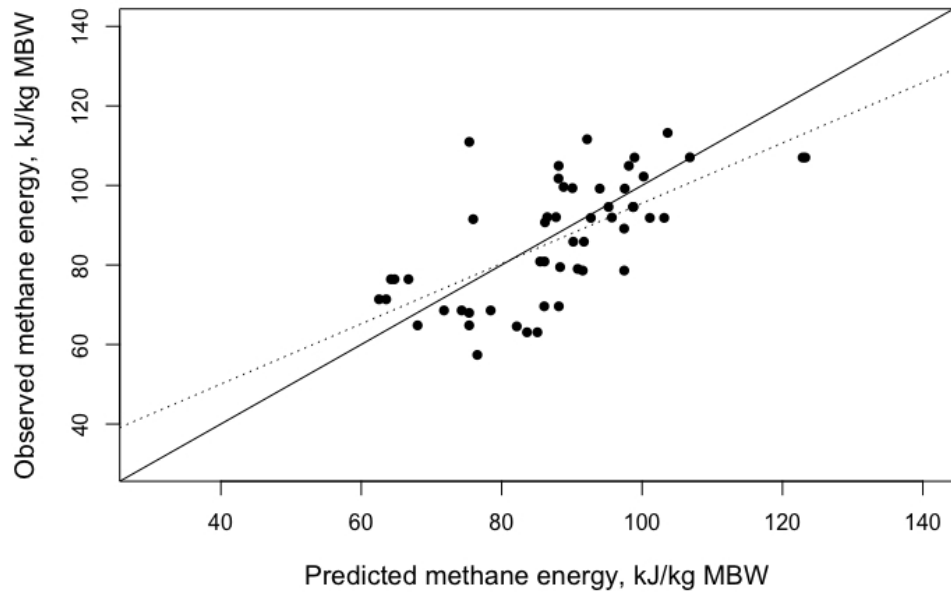


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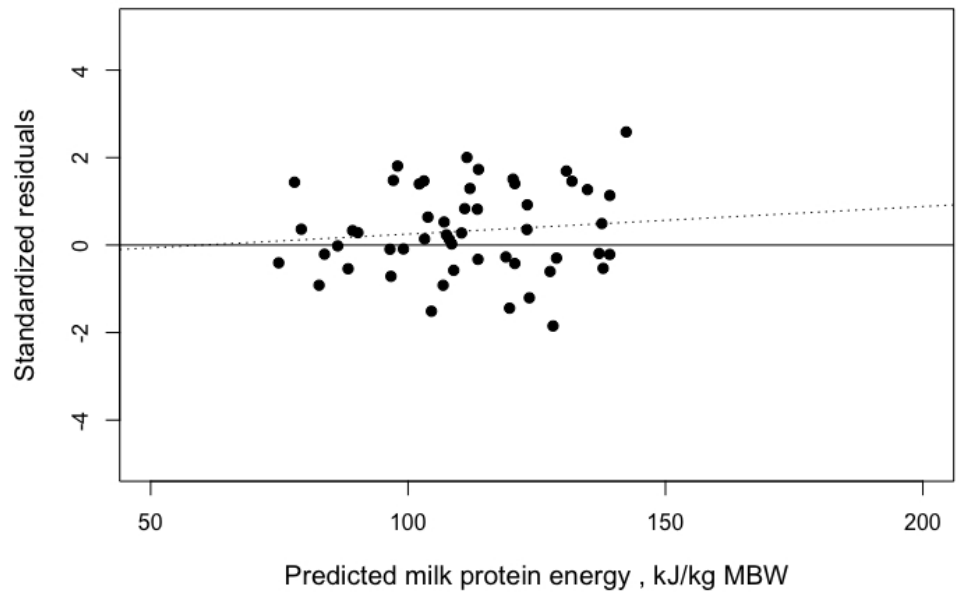
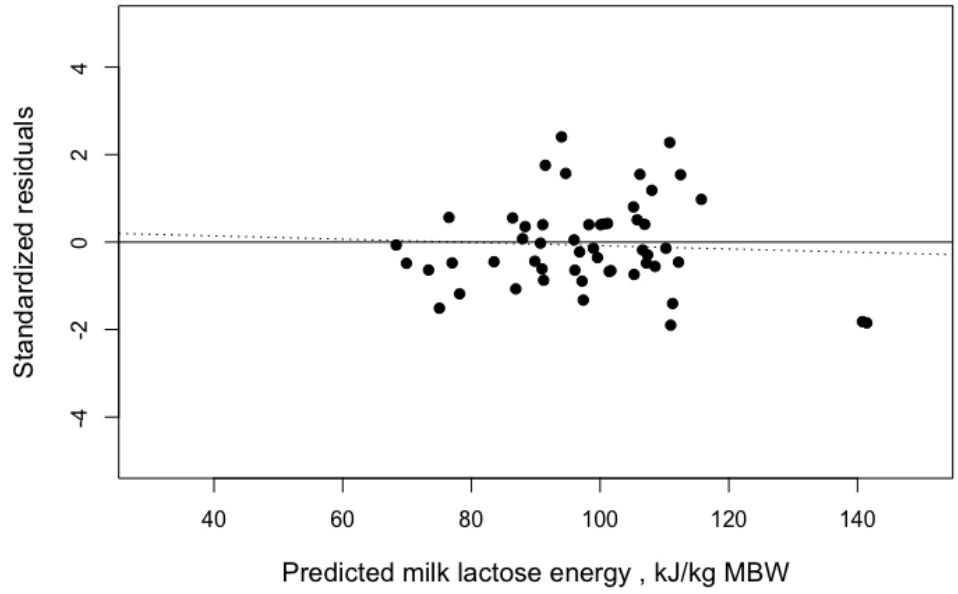
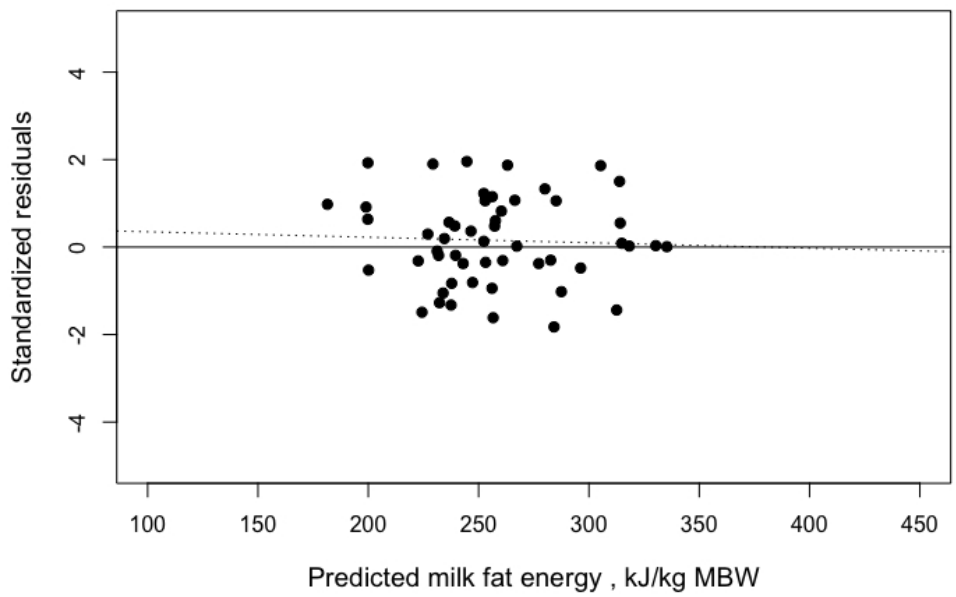


Figure 5. Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model internal evaluation in dairy goats [kJ/kg BW<sup>0.75</sup> day; BW<sup>0.75</sup> = MBW].

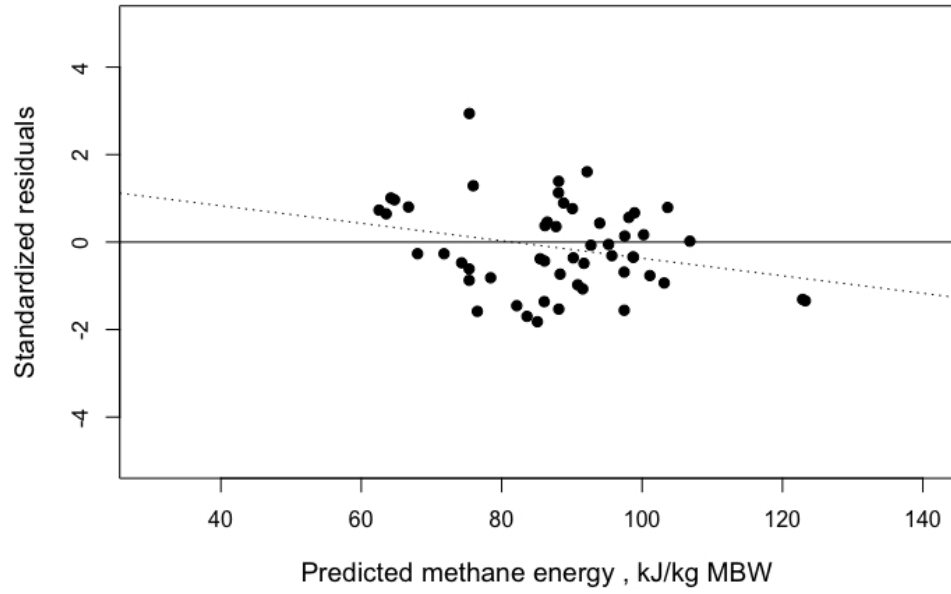
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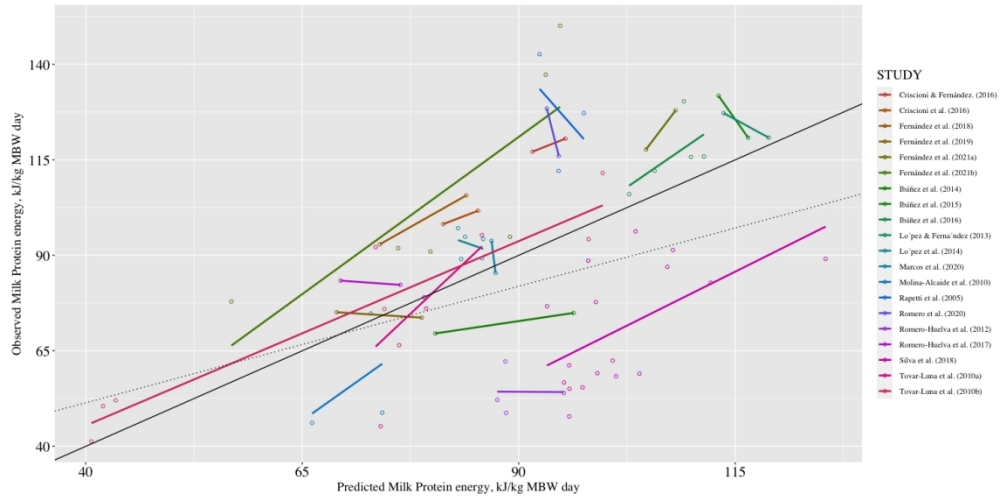
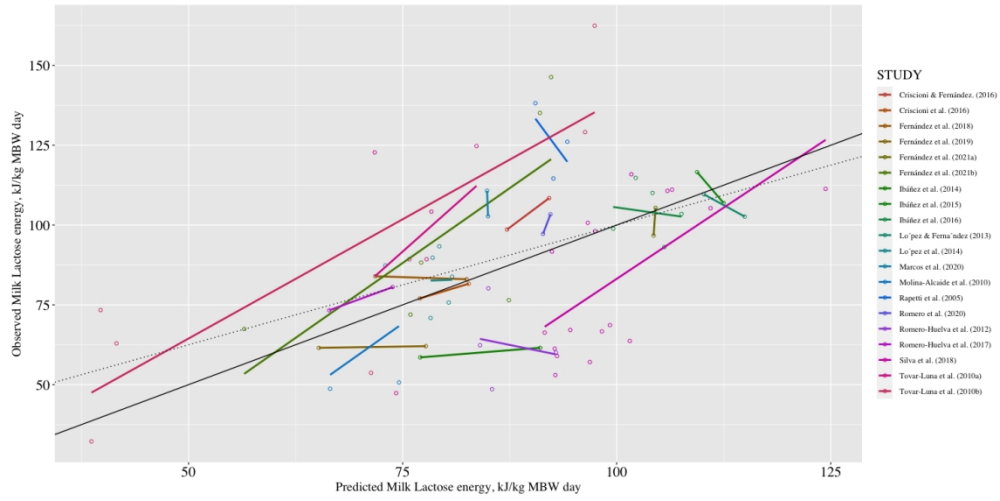
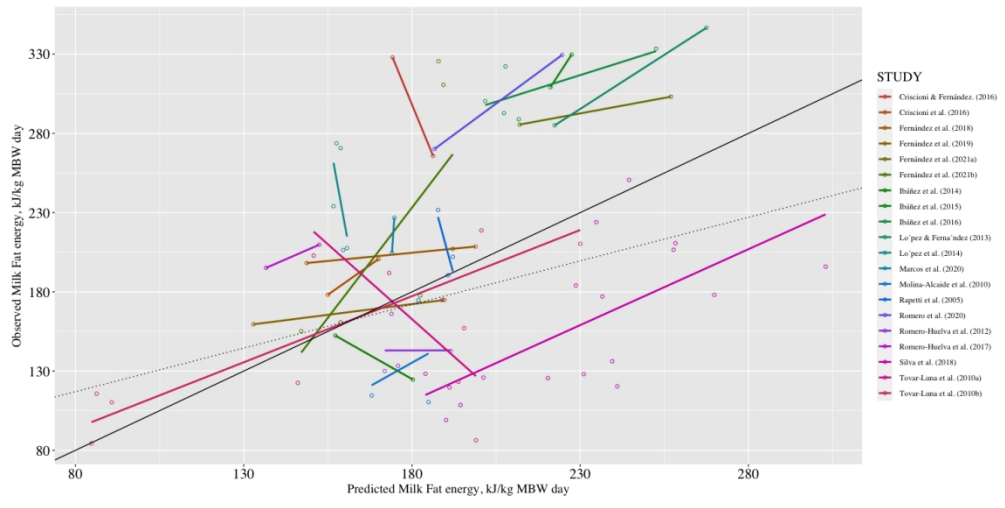


Figure 6. Observed versus predicted values of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model external evaluation in dairy goats [kJ/kg BW0.75 day; BW0.75 = MBW].

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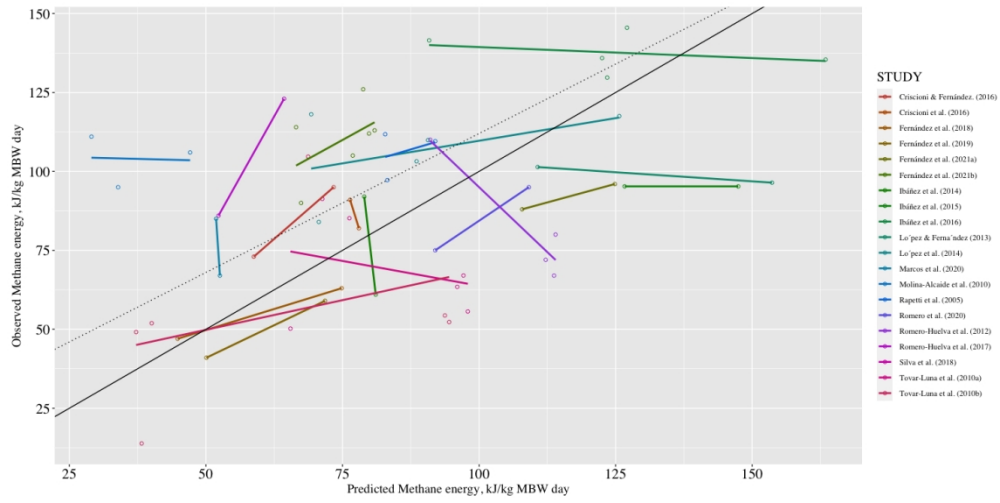


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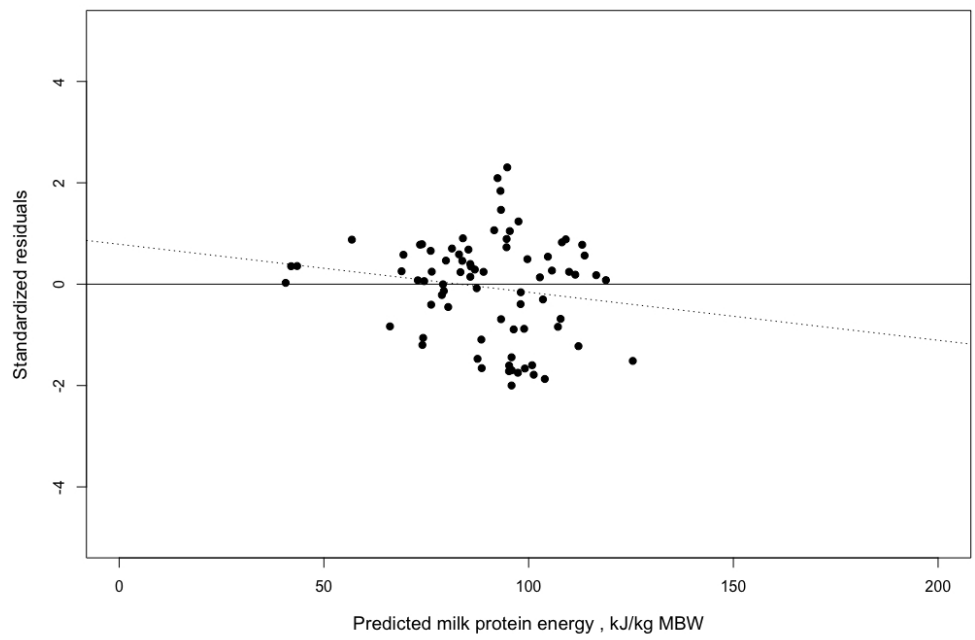
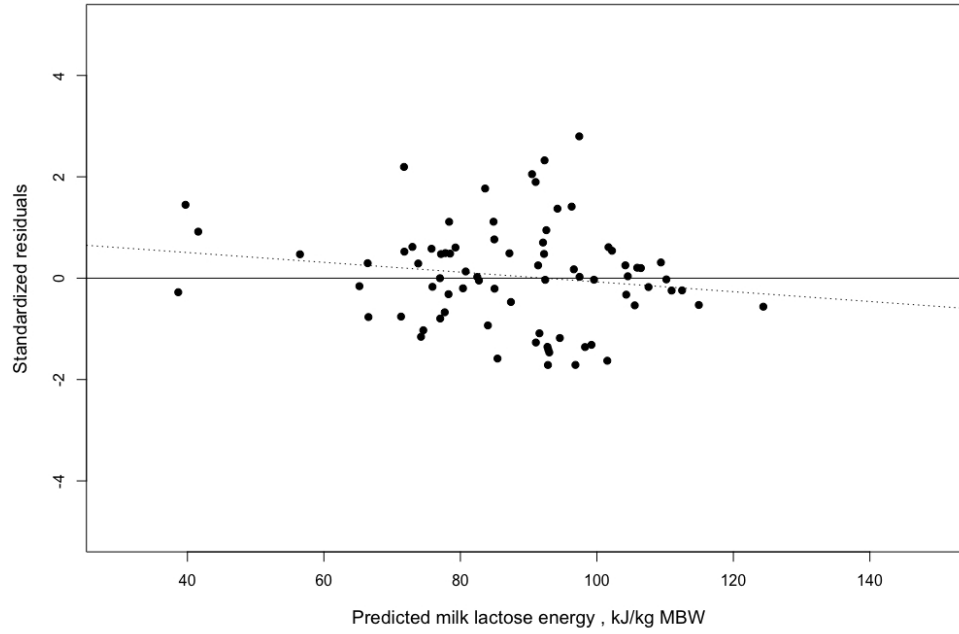
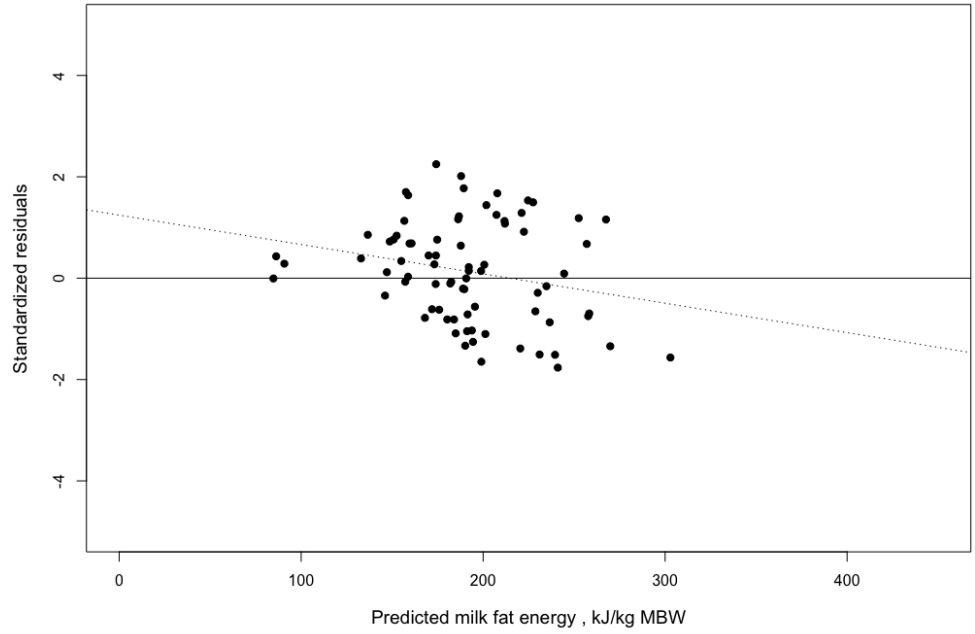


Figure 7. Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model external evaluation in dairy goats [kJ/kg BW0.75 day; BW0.75 = MBW].

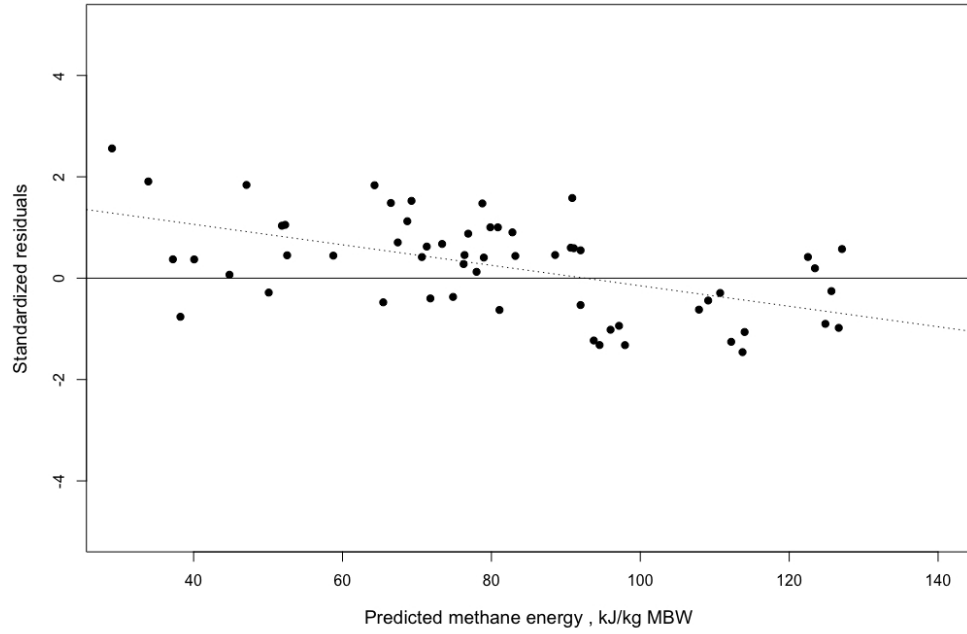
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