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**

4 **Carlos Fernández[†,1] and Juan J. Loor[‡]**

5 [†]Instituto de Ciencia y Tecnología Animal, Universitat Politècnica de Valencia, España.

6 [‡]Department of Animal Sciences, Division of Nutritional Sciences, University of Illinois, USA.

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10 [1] Corresponding author: cjfernandez@dca.upv.es

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Abstract

Feed costs are overwhelmingly the largest expense for dairy producers. Thus, improving

milk production efficiency (milk fat and protein are the main incomes for farmers) is of

great economic importance in the dairy industry. The main objective of this study was to

develop a dynamic energy partitioning model to describe and quantify how dietary energy

from carbohydrate, protein and fat is transferred to milk (protein, lactose and fat) in dairy

goats. In addition, due to increasing worldwide concerns regarding livestock contribution

to global warming, methane (CH_4) emission was quantified. For modeling purposes, 158

individual goat observations were used and randomly split into 2/3 for model

development and 1/3 for internal evaluation. For external evaluation, 20 different energy

balance studies from the literature (77 observations) were evaluated. The Root Mean

Square Prediction Error (RMSPE) was 13.2% for loss of energy in CH_4, 16.8% for energy

in fat, 19.4% for energy in protein and 22.3 energy in lactose. Mean bias was around zero

for all variables and the slope bias was zero for milk energy in lactose, close to 1% for

milk fat (1.01%) and around 3% and 10% for protein and CH_4, respectively. Random bias

was greater than 85% for energy in CH_4 and milk energy components indicating non-

systematic errors and that the equation in the model fitted the data properly. Analyses of

residuals appeared to be randomly distributed around zero. Slopes of regression lines for

residuals versus predicted were positive for milk fat energy, zero for lactose and negative

for milk energy in protein and CH_4. This model suggested for use with mixed diets and

by-products to obtain balanced macronutrient supply, methane emissions and milk

performance during mid lactation could be an interesting tool to help farmers simulate

scenarios that increase milk fat and protein, evaluate CH_4 emissions, without the costs of

running animal trials.

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.

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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.

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

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69   **Abbreviations:** CCC, concordance correlation coefficient; CH_4, methane; E, energy; HP, heat

70   production; Hf, heat of fermentation; HPx, 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

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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_4) emissions. Methane accounts for 14% of total global greenhouse gas

91 emissions and is 28 times more potent than CO_2 (IPCC, 2014). Enteric CH_4 emissions

92 from farmed ruminants account for 25% of total CH_4 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_4 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_4 (around 4.9%

98 of the total CH_4 emissions from livestock). Likewise, future CH_4 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_4 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_4

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_4 emission).

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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

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124   respiration units have been used widely in indirect calorimetry to estimate both heat

125   production and enteric CH_4 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 ± 4.4 kg of BW) and milk

136   production in the previous lactation (630 ± 51 kg of milk per 210 ± 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 × 20 goats × 2 cross-over × 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_4 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 $BW^{0.75}$) represented by the capital

173   letter Q followed with the name of the pool; (1. Gross energy intake [GEI], 2. Protein

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174   intake [PI], 3. Fat intake [FI], 4. Carbohydrate intake [CI], 5. Methane [CH_4], 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 $BW^{0.75}$ 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

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

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

184

$$F_i = k_i \, x \, Q_i$$

185   or

186

$$F_i = k'_i \, x \, Q_i$$

187

$$k'_i = k_i \, x \left(\frac{input}{reference\ constant} \right)^n$$

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

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

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:

$$\frac{dQ\_GEI}{dt} = - F_{GEI\_PI} - F_{GEI\_FI} - F_{GEI\_CI}$$

209

210   Outputs:

$$F_{GEI\_PI} = k_{GEI\_PI} \times Q\_GEI$$

211

$$F_{GEI\_FI} = k_{GEI\_FI} \times Q\_GEI$$

212

$$F_{GEI\_CI} = k_{GEI\_CI} \times Q\_GEI$$

213

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

$$GEI = \int_{t0}^{t} \frac{dQ\_GEI}{dt} + iGEI$$

215

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).

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219 *2.Protein intake pool, Q_PI (kJ/kg BW$^{0.75}$)*. 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
$$PI\ (kJ) = \ DMI(kg) \times \ CP_{diet}\left(\frac{g}{kgDM}\right) \times \ 23.86\left(\frac{kj}{g}\right)$$

224 This expression was divided by the metabolic BW (kg BW$^{0.75}$), 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 $F_{PI\_PA} = k_{PI\_PA}\ x\ Q\_PI$, 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$^{0.75}$)*.

230 Differential equation:

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

232 Input:

233
$$F_{GEI\_PI} = \ k_{GEI\_PI}\ x\ Q\_GEI$$

234 Outputs:

235
$$F_{PI\_feces} = \ k_{PI\_feces}\ x\ Q\_PI$$

236
$$F_{PI\_PA} = \ k_{PI\_PA}\ x\ Q\_PI$$

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

238
$$PI = \int\limits_{t0}^{t}\frac{dQ\_PI}{dt} + iPI$$

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$^{0.75}$).

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

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   *x 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
$$\frac{dQ\_FI}{dt} = \ F_{GEI\_PI} - \ F_{FI\_feces} - \ F_{FI\_PA}$$

254   Input:

255
$$F_{GEI\_FI} = \ k_{GEI\_FI}\ x\ Q\_GEI$$

256   Outputs:

257
$$F_{FI\_feces} = \ k_{FI\_feces}\ x\ Q\_FI$$

258
$$F_{FI\_FA} = \ k_{FI\_FA}\ x\ Q\_FI$$

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

260
$$FI = \ \int_{t0}^{t}\frac{dQ\_FI}{dt} + iFI$$

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$^{0.75}$).

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264   *4.Carbohydrate intake pool, Q_CI (kJ/kg BW$^{0.75}$)*. The carbohydrate intake pool includes

265   one input and three outputs. The amount of carbohydrate intake was determined by

266   difference as follow:

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

268   The GEI was obtained experimentally (2085 kJ/kg BW$^{0.75}$, Table 1) and PI and FI

269   were defined previously. This expression was divided by the metabolic BW (kg BW$^{0.75}$).

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 ($F_{CI\_feces} = k_{CI\_feces} \ x \ Q\_CI$),

272   carbohydrate fermented to VFA ($F_{CI\_VFA} = k_{CI\_VFA} \ x \ Q\_CI$) and carbohydrate that passes

273   to the lower intestinal tract ($F_{CI\_CA} = k_{CI\_CA} \ x \ Q\_CI$). 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$^{0.75}$).*

279   Differential equation:

280    $$\frac{dQ\_CI}{dt} = F_{GEI\_CI} - F_{CI\_feces} - F_{CI\_VFA} - F_{CI\_CA}$$

281   Input:

282    $$F_{GEI\_CI} = k_{GEI\_CI} \ x \ Q\_GEI$$

283   Outputs:

284    $$F_{CI\_feces} = k_{CI\_feces} \ x \ Q\_CI$$

285    $$F_{CI\_VFA} = k_{CI\_VFA} \ x \ Q\_CI$$

286    $$F_{CI\_CA} = k_{CI\_CA} \ x \ Q\_CI$$

287

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

1

289
$$CI = \int_{t0}^{t} \frac{dQ\_CI}{dt} + iCI$$

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 $BW^{0.75}$).

292

293   *5.Methane energy waste pool, Q_CH$_4$ (kJ/kg $BW^{0.75}$)*. The CH_4 pool had one input,

294   F_{VFA_CH4}. The CH_4 pool represents the amount of energy losses to the atmosphere from

295   fermentation in the VFA pool (Q_VFA). The quantities of CH_4 produced by goats were

296   obtained experimentally by an open circuit head-hood indirect calorimetry system. Thus,

297   the fractional rate was calculated as: $k_{VFA\_CH4} = \frac{F_{VFA\_CH4}}{Q\_VFA}$. The CH_4 flux (F_{VFA_CH4}) 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$_4$ energy waste Pool, Q_CH$_4$ (kJ/kg $BW^{0.75}$)*.

303   Differential equation:

304
$$\frac{dQ\_CH4}{dt} = F_{VFA\_CH4}$$

305   Input:

306
$$F_{VFA\_CH4} = k_{VFA\_CH4} \, x \left(\frac{NDF}{30}\right)^{0.011} x \left(\frac{3}{EE}\right)^{0.11} x \, Q\_VFA$$

307   The CH_4 waste energy pool size was expressed by the integral equation:

308
$$CH4 = \int_{t0}^{t} \frac{dQ\_CH4}{dt} + iCH4$$

309   Representing the quantity of energy accumulated from initial time (t_0) to final time

310   (t), with iCH4 being the initial pool size (0 kJ/kg $BW^{0.75}$).

1

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_{CI_VFA} and the output $F_{VFA-CH4}$ 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 × CH$_4$)

323   according to Fahey and Berger (1988). Then, HP from oxidation (HPx) 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   $$F_{VFA\_FA} = (Q\_VFA - F_{VFA\_CH4} - F_{VFA\_Hf}) \; x \; 0.6$$

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   $$F_{VFA\_CA} = Q\_VFA - F_{VFA-CH4} - F_{VFA\_Hf} - F_{VFA\_FA}$$

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

335   Differential equation:

1

336
$$\frac{dQ\_VFA}{dt} = F_{CI\_VFA} - F_{VFA\_CH4} - F_{VFA\_Hf} - F_{VFA\_CA} - F_{VFA\_FA}$$

337 Input:

338
$$F_{CI\_VFA} = k_{CI\_VFA} \; x \; Q\_CI$$

339 Outputs:

340
$$F_{VFA\_CH4} = k_{VFA\_CH4} \; x \left(\frac{NDF}{30}\right)^{0.011} x \left(\frac{3}{EE}\right)^{0.11} x \; Q\_VFA$$

341
$$F_{VFA\_Hf} = k_{VFA\_Hf} \; x \; Q\_VFA$$

342
$$F_{VFA\_CA} = k_{VFA\_CA} \; x \; Q\_VFA$$

343
$$F_{VFA\_FA} = k_{VFA\_FA} \; x \; Q\_VFA$$

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

345
$$VFA = \int_{t0}^{t} \frac{dQ\_VFA}{dt} + iVFA$$

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

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

1

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

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

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

375   Input:

376
$$F_{PI\_PA} = \, k_{PI\_PA} \, x \, Q\_PI$$

377
$$F_{RP\_PA} = \, k_{RP\_PA} \, x \, Q\_RP$$

378   Outputs:

379
$$F_{PA\_MP} = \, k_{PA\_MP} \, x \, Q\_PA$$

380
$$F_{PA\_RP} = \, k_{PA\_RP} \, x \, Q\_PA$$

381
$$F_{PA\_OXP} = k_{PA\_OXP} \; x \; Q\_PA$$

382
$$F_{PA\_UEN} = k_{PA\_UEN} \; x \; Q\_PA$$

383
$$F_{PA\_CA} = k_{PA\_CA} \; x \left(\frac{0.6}{qm}\right) x \; Q\_PA$$

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

385
$$PA = \int_{t0}^{t} \frac{dQ\_PA}{dt} + iPA$$

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 kJ/kg $BW^{0.75}$).

388

389   *8.Fat absorbed pool, Q_FA (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
$$FA \; (kJ) = FI\left(\frac{kJ}{kg \; BW^{0.75}}\right) \times \left(\frac{EE_{digestibility}}{100}\right)$$

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 Knegsel et al., 2007), the flux F_{FA_MF} was

403   corrected by NDF.

1

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

407   This expression was divided by the metabolic BW (kg $BW^{0.75}$). 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        $$F_{FA\_UENfree}(kJ) = UE_{calorimetric\ bomb}\ (kJ) - F_{PA\_UEN}$$

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 $BW^{0.75}$).

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 $BW^{0.75}$).*

417   Differential equation:

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

419   Input:

420        $$F_{FI\_FA} = k_{FI\_FA}\ x\ Q\_FI$$

421        $$F_{VFA\_FA} = k_{VFA\_FA}\ x\ Q\_VFA$$

422        $$F_{CA\_FA} = k_{CA\_FA}\ x \left(\frac{0.6}{qm}\right) x\ Q\_CA$$

423        $$F_{RF\_FA} = k_{RF\_FA}\ x\ Q\_RF$$

424   Outputs:

425
$$F_{FA\_MF} = k_{FA\_MF} \, x \left(\frac{NDF}{30}\right)^{0.01} x \, Q\_FA$$

426
$$F_{FA\_RF} = k_{FA\_RF} \, x \, Q\_FA$$

427
$$F_{FA\_OXF} = k_{FA\_OXF} \, x \left(\frac{0.6}{qm}\right) x \, Q\_FA$$

428
$$F_{FA\_UENfree} = k_{FA\_UENfree} \, x \, Q\_FA$$

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

430
$$FA = \int_{t0}^{t} \frac{dQ\_FA}{dt} + iFA$$

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$^{0.75}$).

433

434   *9.Carbohydrate absorbed pool, Q_CA (kJ/kg BW$^{0.75}$)*. The carbohydrate absorbed pool

435   includes three inputs and four outputs. The amount of carbohydrate absorbed was

436   determined as follows:

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

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 glucogenesis (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}).

1

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

449   This expression was divided by the metabolic BW (kg $BW^{0.75}$). 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     $$F_{CA\_UENfree}(kJ) = UE_{calorimetric\,bomb}\,(kJ) - F_{PA\_UEN}$$

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 $BW^{0.75}$).

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 $BW^{0.75}$).*

459   Differential equation:

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

461   Input:

462     $$F_{CI\_CA} = k_{CI\_CA}\,x\,Q\_CI$$

463     $$F_{VFA\_CA} = k_{VFA\_CA}\,x\,Q\_VFA$$

464     $$F_{PA\_CA} = k_{PA\_CA}\,x\left(\frac{0.6}{qm}\right)x\,Q\_PA$$

465   Outputs:

466     $$F_{CA\_ML} = k_{CA\_ML}\,x\,Q\_CA$$

467     $$F_{CA\_FA} = k_{CA\_FA}\,x\left(\frac{0.6}{qm}\right)x\,Q\_CA$$

468
$$F_{CA\_OXC} = k_{CA\_OXC} \, x \left(\frac{qm}{0.6}\right) x \, Q\_CA$$

469
$$F_{CA\_UENfree} = k_{CA\_UENfree} \, x \, Q\_CA$$

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

471
$$CA = \int_{t0}^{t} \frac{dQ\_CA}{dt} + iCA$$

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$^{0.75}$).

474

475   *10.Protein retention pool, Q_RP (kJ/kg BW$^{0.75}$)*. The protein-retained pool includes one

476   input and one output. The amount of protein retained was determined as follows:

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

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

481   Differential equation:

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

483   Input:

484
$$F_{PA\_RP} = \ k_{PA\_RP} \, x \, Q\_PA$$

485   Outputs:

486
$$F_{RP\_FA} = \ k_{RP\_FA} \, x \, Q\_RP$$

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

488
$$RP = \int_{t0}^{t} \frac{dQ\_RP}{dt} + iRP$$

2

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 kJ/kg $BW^{0.75}$, see Table 1).

491

492   *11.Fat retention pool, Q_RF (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    $$RF \ (kJ) = RE \ (kJ) - RP \ (kJ)$$

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 (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    $$\text{if} \ (qm \geqq 0.6)$$

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

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

508    $$\text{else}$$

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

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

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
$$\frac{dQ\_RF}{dt} = F_{FA\_RF} - F_{RF\_FA}$$

518 Input:

519
$$F_{FA\_RF} = k_{FA\_RF} \, x \, Q\_FA$$

520 Outputs:

521
$$F_{RF\_FA} = k_{RF\_FA} \, x \, Q\_RF$$

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

523
$$RF = \int_{t0}^{t} \frac{dQ\_RF}{dt} + iRP$$

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
$$MP = MY \left(\frac{g}{d}\right) x \, Milk \, Protein \left(\frac{g}{100g}\right) x \, 23.64 \left(\frac{kJ}{g}\right)$$

533   Where MY was milk production and this expression was divided by the metabolic

534 BW (kg BW$^{0.75}$).

2

535   *Milk protein energy Pool, Q_MP (kJ/kg BW$^{0.75}$).*

536   Differential equation:

537
$$\frac{dQ\_MP}{dt} = F_{PA\_MP}$$

538   Input:

539
$$F_{PA\_MP} = k_{PA\_MP} \; x \; Q\_PA$$

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

541
$$MP = \int_{t0}^{t} \frac{dQ\_MP}{dt} + iMP$$

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$^{0.75}$).

544

545   *13.Milk lactose energy pool, Q_ML (kJ/kg BW$^{0.75}$).* 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
$$ML = MY \left(\frac{g}{d}\right) x \; Milk \; Lactose \left(\frac{g}{100g}\right) x \; 17.36 \left(\frac{kJ}{g}\right)$$

551   Where MY was milk production and this expression was divided by the metabolic

552   BW (kg BW$^{0.75}$).

553   *Milk lactose energy Pool, Q_ML (kJ/kg BW$^{0.75}$).*

554   Differential equation:

555
$$\frac{dQ\_ML}{dt} = F_{CA\_ML}$$

556   Input:

557
$$F_{CA\_ML} = k_{CA\_ML} \; x \; Q\_CA$$

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

559
$$ML = \int_{t0}^{t} \frac{dQ\_ML}{dt} + iML$$

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$^{0.75}$).

562

563 *14.Milk fat energy pool, Q_MF (kJ/kg BW$^{0.75}$).* 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
$$MF = MY \left(\frac{g}{d}\right) x \; Milk \; Fat \left(\frac{g}{100g}\right) x \; 39.33 \left(\frac{kJ}{g}\right)$$

568 Where MY was milk production and this expression was divided by the metabolic

569 BW (kg BW$^{0.75}$).

570 *Milk fat energy Pool, Q_ML (kJ/kg BW$^{0.75}$).*

571 Differential equation:

572
$$\frac{dQ\_MF}{dt} = F_{FA\_MF}$$

573 Input:

574
$$F_{FA\_MF} = k_{FA\_MF} \, x \left(\frac{NDF}{30}\right)^{0.01} x \; Q\_FA$$

575

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

577
$$MF = \int_{t0}^{t} \frac{dQ\_MF}{dt} + iMF$$

2

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 $BW^{0.75}$).

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_4 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$_4$

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_4 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_CH4} 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_4, 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_4 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_4, respectively. Random bias was greater than 85% for energy in CH_4

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 $BW^{0.75}$ 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 $BW^{0.75}$ per day

651 (Figure 2c), and below this range it overestimated and above it underestimated. For

652 energy in CH_4 with a narrow range about 80-90 kJ/kg $BW^{0.75}$ 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_4

655   was off by 23.08, 22.22, 43.84 and 11.36 kJ/kg $BW^{0.75}$ 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_4 (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_4, 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_4 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_4. The slope bias was

673   lower for ML and MF (0.84% and 2.54%, respectively) and greater for CH_4 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_4 (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 he 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_4 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_4 was off by 19.83, 22.87, 49.63 and 11.77 kJ/kg $BW^{0.75}$ 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_4 (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_4.

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_4 was not calculated

697 because some literature experiments did not determine CH_4 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_4 (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_4 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_4 are

706 shown in Figure 6. This figure includes 20 data sets from energy balance experiments

707 form 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 grater values and in CH_4 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_4 (Figure 5a, 5b, 5c and 5d,

714 respectively), being less accurate for extreme values.

715

Discussion

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_4 emissions, milk and loss of heat when daily

3

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_4 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_4 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_4 were available. The CH_4 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_4 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_4 emissions were observed among

789   diets for observed and model prediction, but on average the model estimated 45 kJ/kg

790      $BW^{0.75}$ lower emission than observed. The challenge in quantifying CH_4 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_4 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_4 was observed and the model adjusted better. The

802   presence of plant secondary compounds in by-products may promote less CH_4 production

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

804   Fernández et al. (2021b) studied the CH_4 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_4

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     $BW^{0.75}$, 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 $BW^{0.75}$ (total energy of

828   434 kJ/kg $BW^{0.75}$ similar to the value observed; 444 kJ/kg $BW^{0.75}$), 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 $BW^{0.75}$ and the

831   predicted was 255 kJ/kg $BW^{0.75}$. 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 $BW^{0.75}$) 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 $BW^{0.75}$ 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_4 was 96 kJ/kg $BW^{0.75}$, 16 kJ/kg $BW^{0.75}$ 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 $BW^{0.75}$, respectively (observed values were 76, 104 and 157

846   kJ/kg $BW^{0.75}$, respectively). The model predicted storage of body energy as fat of 151

847   kJ/kg $BW^{0.75}$, and an energy wasted in CH_4 of 68 kJ/kg $BW^{0.75}$ (the observed value was

848   56 kJ/kg $BW^{0.75}$). 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 $BW^{0.75}$ (from PA to CA pool), and the transfer from the carbohydrate to the fat

855   pool was 474 kJ/kg $BW^{0.75}$ (from CA to FA pool). The daily accretion of fat reserves was

856   -33 kJ/kg $BW^{0.75}$, (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_4 was 112, 78, 212 and 68 kJ/kg $BW^{0.75}$ (close to the observed

860   values 95, 125, 192 and 85 kJ/kg $BW^{0.75}$, respectively), respectively. Thus, total milk

861   energy predicted was 402 kJ/kg $BW^{0.75}$ and the observed 412 kJ/kg $BW^{0.75}$. 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 $BW^{0.75}$ 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 $BW^{0.75}$

866   and day), indicating accumulation of fat.

867   Although theorical daily simulation of gluconeogenesis was similar between diets

868   (44 kJ/kg $BW^{0.75}$), lipogenesis was 52 kJ/kg $BW^{0.75}$ 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 Knegsel 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 $BW^{0.75}$ vs

877   242 kJ/kg $BW^{0.75}$) and 37 kJ/kg $BW^{0.75}$ 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_4 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_4 predicted and observed, for the control diet, was 22 and 26 g/d,

910   respectively. The CH_4 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 qm = 0.61 and the byproduct diet a qm = 0.54. For the qm = 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 qm (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 qm = 0.61 had greater oxidation of carbohydrate than fat (47% vs

945 35%), and in the group with a lower qm 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 qm; when the qm was high, the energy oxidized

948 from carbohydrate was higher than from fat oxidation and when the qm 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 qm high and low respectively). Therefore, when the qm

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 kJ/kg $BW^{0.75}$

957   lower for the diet with qm = 0.61 than the diet with qm = 0.54. Thus, when qm 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 kJ/kg $BW^{0.75}$ (difference between

963   F_{FA_RF} and F_{RF_FA}) highlighting that in the diet with lower qm 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

4

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 $BW^{0.75}$

1162 day; $BW^{0.75}$ = 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 $BW^{0.75}$ day; $BW^{0.75}$ =

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

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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)

Variable[1]	Mean	Min.	Max.	SD
Lactating Dairy Goat fed Mixed Diet				
Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	70	67	72	1.9
EE	67	53	76	8.3
Energy	67	54	79	5.2
Energy partitioning (kJ/kg $BW^{0.75}$ per day)				
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

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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
Nitrogen balance (g/day)				
Urinary nitrogen	20	10	35	6.7
Retained nitrogen	3	-3	8	3.6
Goat characteristics				
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

[1] 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[1]	Mean	Min.	Max.	SD
Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	69	66	72	1.9
EE	67	54	75	9.1
Energy	68	59	77	4.9

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Energy partitioning (kJ/kg BW$^{0.75}$ 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

[1] 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$^{0.75}$)	
Q_GEI	Energy intake
Q_PI	Protein intake
Q_CI	Carbohydrate intake
Q_FI	Fat intake

Q_VFA	Volatile fatty acids
Q_CH$_4$	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

Energy fluxes (kJ/kg BW$^{0.75}$ per hour)

F_{GEI_PI}	energy intake from diet protein
F_{GEI_CI}	energy intake from diet carbohydrate
F_{GEI_FI}	energy intake from diet fat
F_{PI_feces}	energy lost in feces from protein intake
F_{PI_PA}	energy absorbed from protein
F_{CI_feces}	energy lost in feces from carbohydrate intake
F_{CI_CA}	energy absorbed from carbohydrates
F_{CI_VFA}	carbohydrate fermentation to volatile fatty acids
F_{FI_feces}	energy lost in feces from fat intake
F_{FI_FA}	energy absorbed from fat
F_{VFA_CA}	volatile fatty acids to carbohydrate absorbed pool
F_{VFA_FA}	volatile fatty acids to fat absorbed pool
F_{VFA_CH4}	methane production
F_{VFA_Hf}	heat of fermentation
F_{PA_RP}	protein retention
F_{PA_MP}	protein in milk
F_{PA_UEN}	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

Fractional rates (/hour)

k_{GEI_PI}	fractional rate of F_{GEI_PI}
k_{GEI_CI}	fractional rate of F_{GEI_CI}
k_{GEI_FI}	fractional rate of F_{GEI_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_OXP}	fractional rate of F_{PA_OXP}
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}

Reference constants

HP	heat production
HPx	heat production form oxidation of nutrients
Hf	heat of fermentation
OXP	oxidation of protein
OXC	oxidation of carbohydrates
OXF	oxidation of fat

Inputs

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$^{0.75}$ 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[1]	Initial Values	Final Values	SD	CV (%)
k_{VFA_CH4}	0.142	0.110	0.0226	18
k_{PA_MP}	0.575	0.567	0.0057	1
k_{CA_ML}	0.073	0.075	0.0014	2
k_{FA_MF}	0.034	0.030	0.0028	9
Others Paremeters		Fractional rates (/hour)		
k_{GEI_PI}	0.25	F_{GEI_PI} / Q_GEI		mass action kinetics
k_{GEI_CI}	0.69	F_{GEI_CI} / Q_GEI		mass action kinetics
k_{GEI_FI}	0.06	F_{GEI_FI} / Q_GEI		mass action kinetics
k_{PI_feces}	0.30	F_{PI_feces} / Q_PI		mass action kinetics
k_{PI_PA}	0.70	F_{PI_PA} / Q_PI		mass action kinetics
k_{CI_feces}	0.05	F_{CI_feces} / Q_CI		mass action kinetics
k_{CI_CA}	0.36	F_{CI_CA} / Q_CI		mass action kinetics
k_{CI_VFA}	0.60	F_{CI_VFA} / Q_CI		mass action kinetics

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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$^{0.75}$)	Pools (initial values)	Equations	
Q_GEI	2085	(DMI x GE$_{diet}$)/BW$^{0.75}$	
Q_PI	0	[(DMI x CP)/BW$^{0.75}$] x 23.86	
Q_CI	0	GEI - PI - FI	
Q_FI	0	[(DMI x EE)/BW$^{0.75}$] x 39.76	
Q_VFA	0	70% of MEI is supplied as VFA	Demeyer (1992)
Q_CH$_4$	0	observed from indirect calorimetry system	
Q_PA	0	CI x CP$_{digestibility\ coefficient}$	
Q_CA	0	DE$_{intake}$ - PA - FA	
Q_FA	0	FI x EE$_{digestibility\ coefficient}$	
Q_RP	28	[(N retained)/BW$^{0.75}$] x 6.25 x 23.86	
Q_RF	66	RE - RP	
Q_MP	0	[MY x CP$_{milk}$ x 23.64]/BW$^{0.75}$	
Q_ML	0	[MY x Lactose$_{milk}$ x 17.36]/BW$^{0.75}$	
Q_MF	0	[MY x Fat$_{milk}$ x 39.33]/BW$^{0.75}$	

Reference constants

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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	$[(1.719x\ O_2 + 1.719 \times CO_{2x} - 1.963 \times N_{urine}) \times 39.76]/BW^{0.75}$	Brouwer (1958); Chwalibog et al. (1997a)
Inputs			
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 $BW^{0.75}$ per day)	1222	$MEI = GEI - E_{feces} - E_{urine} - E_{CH4}$	
qm	0.60	MEI/GEI	AFRC (1993); INRA (2018)

6

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[1] Parameters abbreviation is given in Table 2.

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

Variable[1] (kJ/kg BW$^{0.75}$ per day)	Mean	Min.	Max.	SD
Lactating Dairy Goat fed Mixed Diet				
Rapetti et al. (2005)				
Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	68	64	72	4.1
EE	78	72	83	5.3
Energy partitioning				
GEI	1916	1877	1940	33.5
Energy in methane	106	97	112	7.8
MEI	1186	1140	1261	65.7
Enery 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
Goat characteristics				
DMI (g/day)	2170	2054	2354	161.4

6

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)

Diet Composition (%DM)

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

Apparent digestibility (%)

CP	68	61	74	5
EE	-	-	-	-

Energy partitioning

GEI	1638	1486	1731	83.4
Energy in methane	69	50	91	16.3
MEI	905	753	1073	109.5
Enery 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

Goat characteristics

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)

Diet Composition (%DM)

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
Apparent digestibility (%)				
CP	75	70	79	3.8
EE	-	-	-	-
Energy partitioning				
GEI	1330	797	2025	588.2
Energy in methane	54	14	105	29.0
MEI	845	540	1231	326.9
Enery 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
Goat characteristics				
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)				
Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	71	69	72	1.4
EE	74	70	80	5.3

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Energy partitioning

GEI	1467	1370	1520	83.9
Energy in methane	104	95	111	8.2
MEI	848	781	899	60.5
Enery 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
Enery in milk	239	229	251	9.9
Energy in milk protein	54	49	62	5.7

7

Energy in milk lactose	63	49	80	13.1
Energy in milk fat	143	130	166	16.3
Goat characteristics				
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
Enery 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

7

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
Enery 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

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qm	0.69	0.65	0.72	0.026
Apparent digestibility (%)				
CP	70	65	75	3.6
EE	72	70	75	2.5
Energy partitioning				
GEI	1649	1629	1668	18.4
Energy in methane	107	84	118	14.0
MEI	1139	1079	1193	46.5
Enery 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
Goat characteristics				
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)

Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	77	76	78	1.4
EE	85	84	86	1.4
Energy partitioning				
GEI	2328	2286	2370	58.9

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Energy in methane	95	95	95	0.0
MEI	1423	1411	1435	16.8
Enery 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

Goat characteristics

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

<div align="center">Criscioni et al. (2016)</div>

Diet Composition (%DM)

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

Apparent digestibility (%)

CP	71	69	74	3.4
EE	61	58	65	4.7

Energy partitioning

GEI	1650	1591	1709	83.4
Energy in methane	87	82	91	6.4
MEI	1089	1085	1092	4.9
Enery 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

7

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
Enery 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

Apparent digestibility (%)

CP	61	56	66	3,5
EE	61	34	74	16

Energy partitioning

GEI	2174	2056	2296	87.9
Energy in methane	138	130	146	6.1
MEI	1352	1311	1412	47.2
Enery 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

Goat characteristics

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 (%)

7

CP	80	79.0	81.0	1.3
EE	-	-	-	-

Energy partitioning

GEI	1440	1360	1520	113.1
Energy in methane	105	86	123	26.2
MEI	957	930	984	38.2
Enery 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

Goat characteristics

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)

Diet Composition (%DM)

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

Apparent digestibility (%)

CP	81	79	83	1.8
EE	-	-	-	-

Energy partitioning

GEI	2109	1906	2662	191.6
Energy in methane	-	-	-	-
MEI	1210	1054	1417	75.9

7

Enery 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
Goat characteristics				
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)

Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	70	66	73	5.0
EE	70	68	73	3.3
Energy partitioning				
GEI	1588	1462	1713	177.5
Energy in methane	55	47	63	11.3
MEI	998	970	1025	38.9
Enery 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
Goat characteristics				
DMI (g/day)	1600	1500	1700	141.4

7

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)

Diet Composition (%DM)

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

Apparent digestibility (%)

CP	69	67	72	4.0
EE	63	57	70	9.6

Energy partitioning

GEI	1477	1334	1620	202.2
Energy in methane	50	41	59	12.7
MEI	951	947	954	4.9
Enery 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

Goat characteristics

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)

Diet Composition (%DM)

CP (%)	16.7	16.0	17.4	0.99
NDF (%)	20.7	20.5	20.8	0.21

8

EE (%)	3.8	2.8	4.7	1.33
GE (MJ/kgDM)				
qm	0.65	0.65	0.66	0.008
Apparent digestibility (%)				
CP	61	46	75	20.7
EE				
Energy partitioning				
GEI	1730	1730	1730	0.0
Energy in methane	76	67	85	12.7
MEI	1130	1120	1140	14.1
Enery 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
Goat characteristics				
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)			
Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	69	67	72	3.1
EE	65	53	76	16.3

8

Energy partitioning

GEI	1926	1913	1939	18.38
Energy in methane	85	75	95	14.1
MEI	1138	1095	1180	60.1
Enery 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
Enery in milk	461	446	476	21.2
Energy in milk protein	123	118	128	7.2

8

Energy in milk lactose	101	97	105	6.1
Energy in milk fat	294	286	303	12.4
Goat characteristics				
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)

Diet Composition (%DM)				
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
Apparent digestibility (%)				
CP	69	66	72	2.2
EE	52	42	61	6.9
Energy partitioning				
GEI	1671	1216	1906	259.3
Energy in methane	110	90	126	11.9
MEI	994	629	1196	215.9
Enery 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
Goat characteristics				
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

8

[1] CP = crude protein; EE = ether extract; GE = gross energy; qm = metabolizability; GEI = gross energy intake; MEI = metabolizable energy intake; DMI = dry matter intake.

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$^{0.75}$ per day)

Variable	Observed mean	Predicted mean	RMSPE[1], %	Mean bias, %	Slope bias, %	Random bias, %	CCC[2]
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

[1] RMSPE = root mean square prediction error as a percentage of observed mean.

[2] CCC = Concordance Correlation Coefficient.

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$^{0.75}$ per day)

Variable	Observed mean	Predicted mean	RMSPE[1], %	Mean bias, %	Slope bias, %	Random bias, %	CCC[2]
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

[1] RMSPE = root mean square prediction error as a percentage of observed mean.

[2] CCC = Concordance Correlation Coefficient.

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 $BW^{0.75}$ per day)

Variable	Observed mean	Predicted mean	RMSPE[1], %	Mean bias, %	Slope bias, %	Random bias, %	CCC[2]
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 | - |

[1] RMSPE = root mean square prediction error as a percentage of observed mean.

[2] CCC = Concordance Correlation Coefficient.

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1312
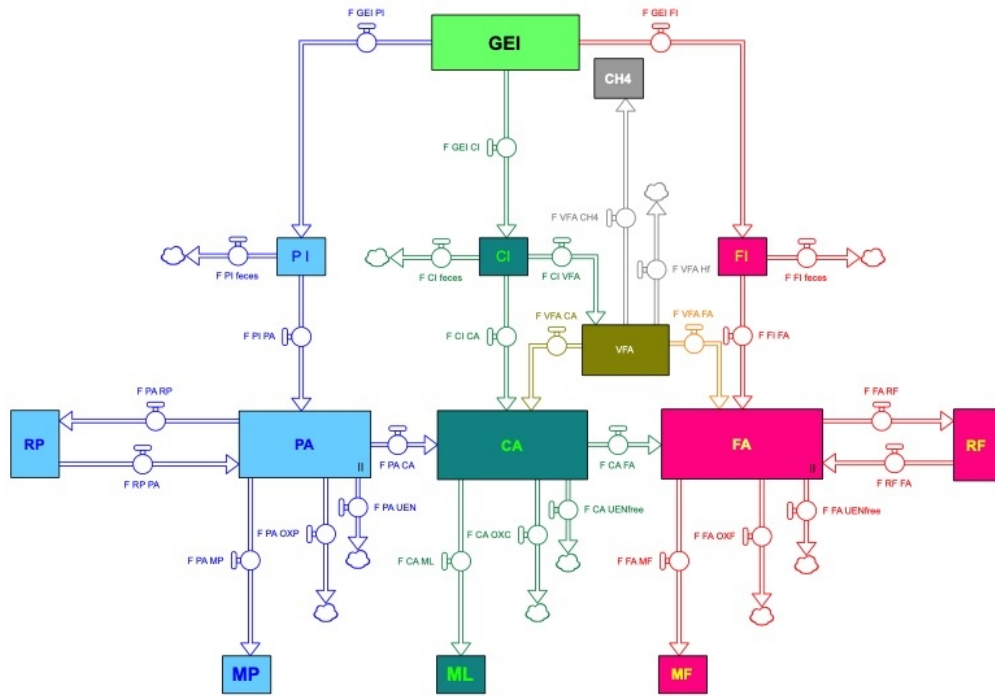
Figure 1. Diagrammatic representation of the energy partitioning mathematical model in dairy goats (using Stella Architect software). See Table 2 for legend.

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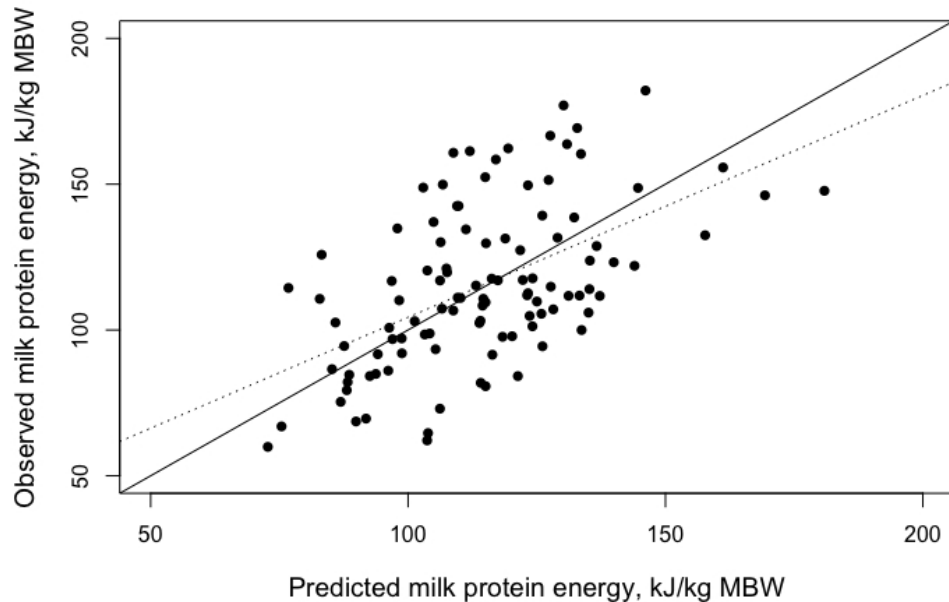
Figure 2. Observed versus predicted values of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model development in dairy goats [kJ/kg BW0.75 day; BW0.75 = MBW]. The regression equations were as follow: milk protein energy Y = 28.27 + 0.76X (standard error = 13.36 and 0.11 for the intercept and slope respectively; residual standard error = 23.08; R2 = 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; R2 = 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; R2 = 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; R2 = 0.42).

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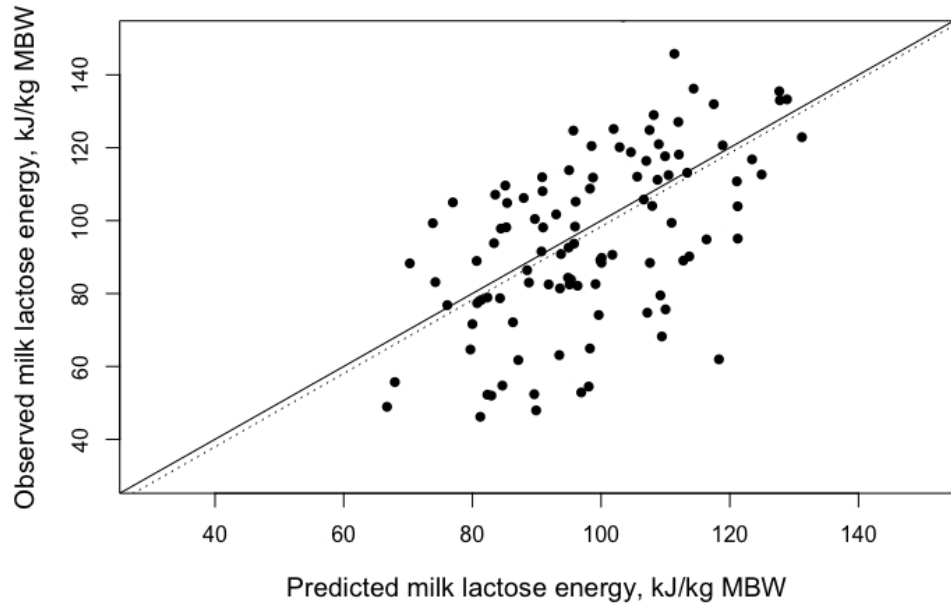
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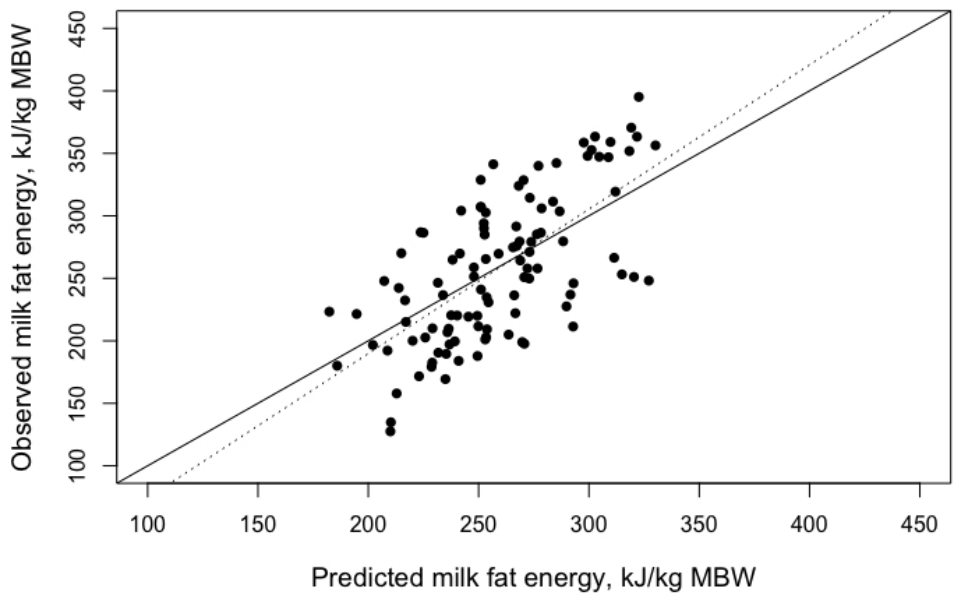
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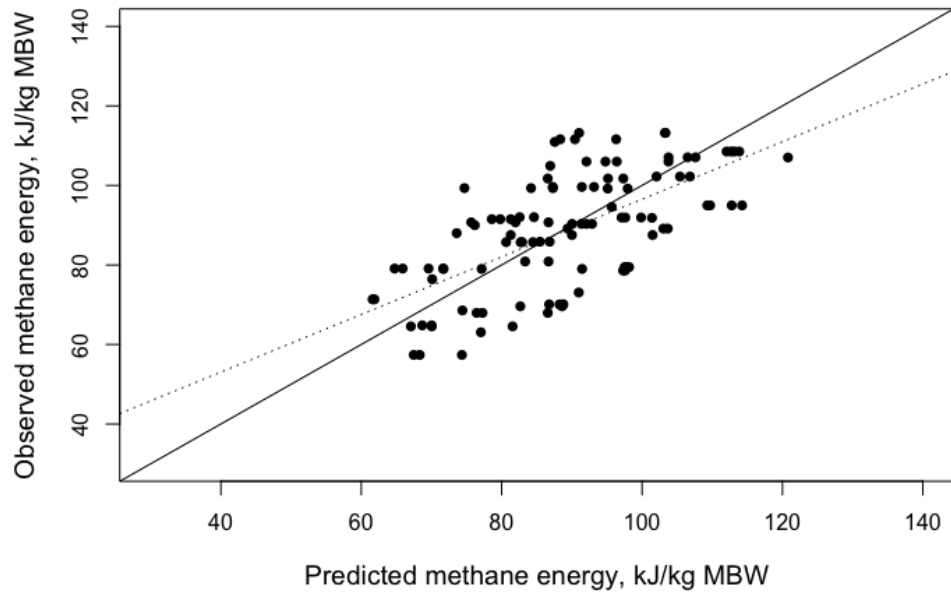
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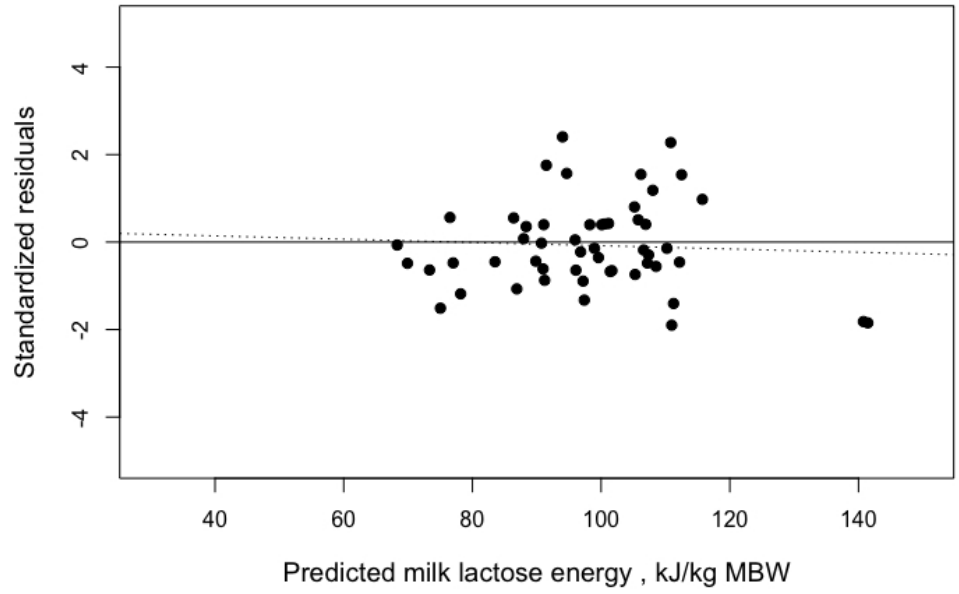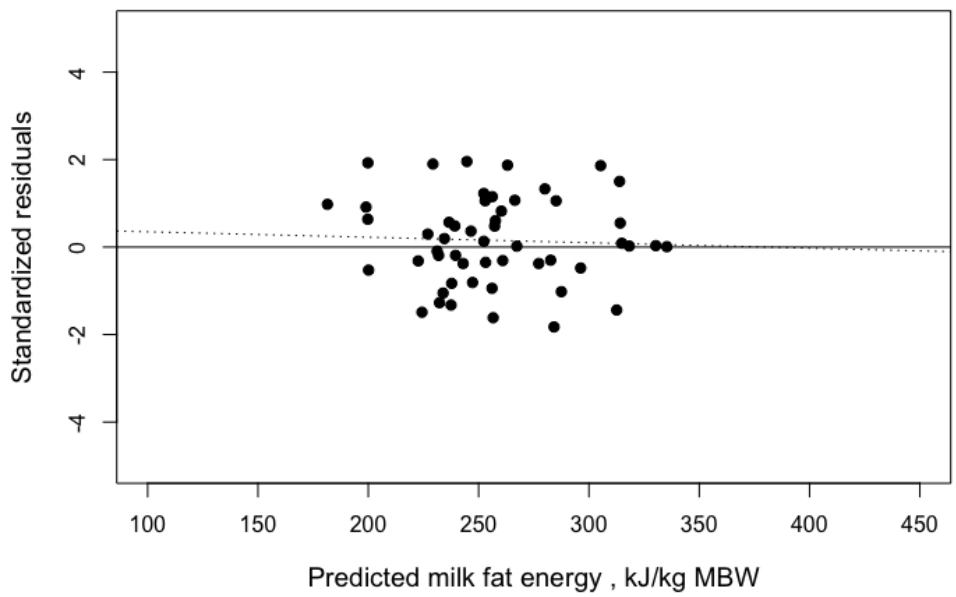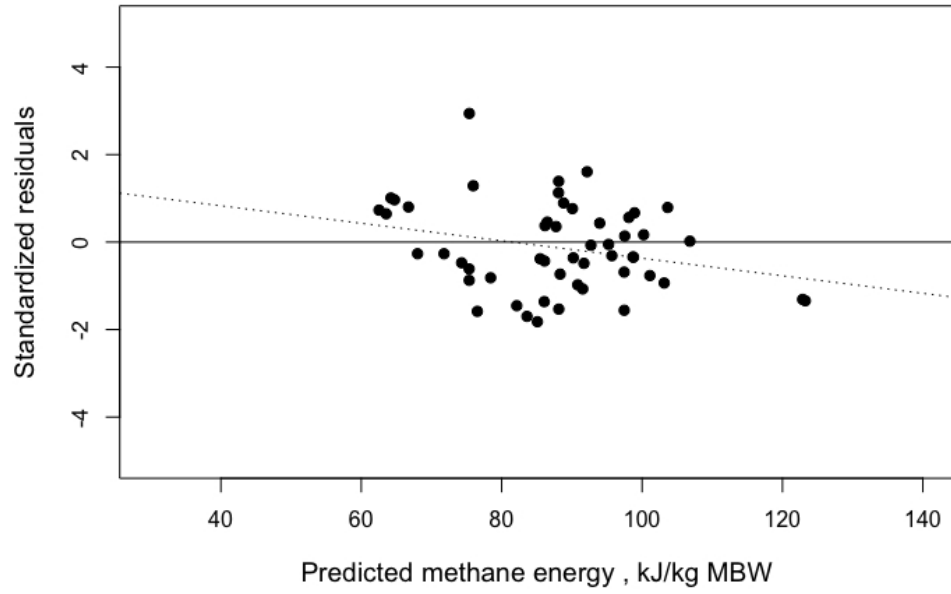
Figure 3. Residuals plot of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model development in dairy goats [kJ/kg BW0.75 day; BW0.75 = MBW].

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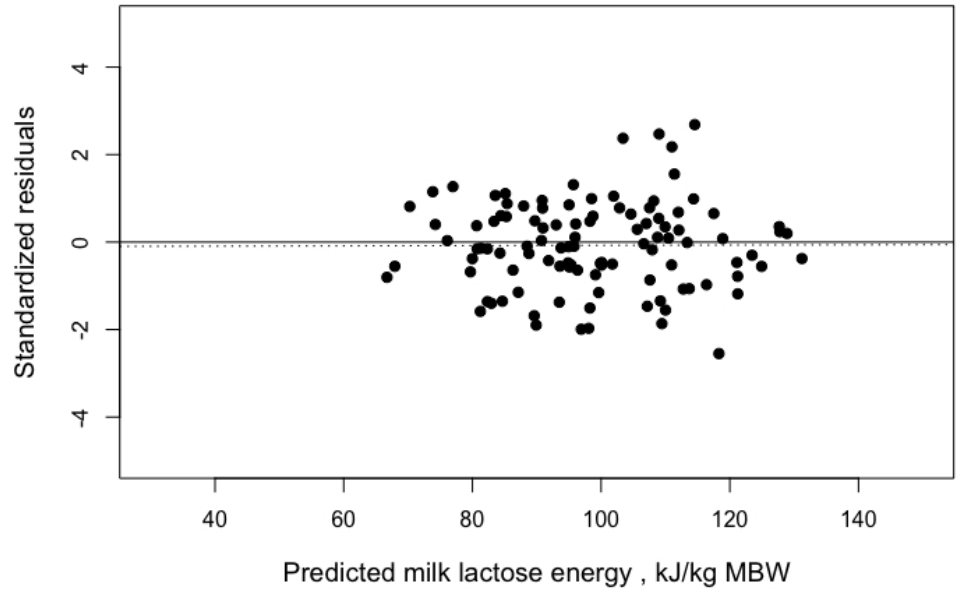
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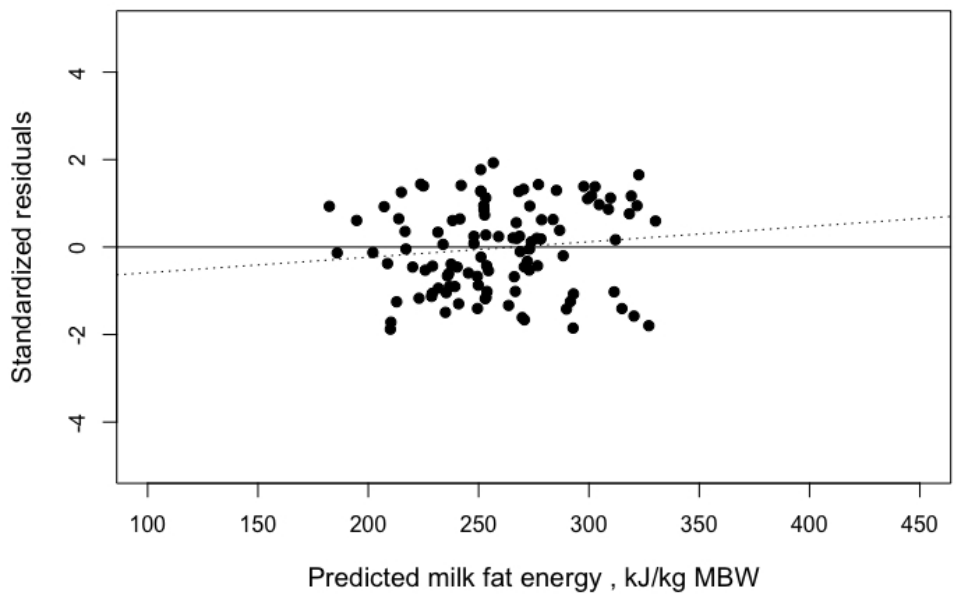
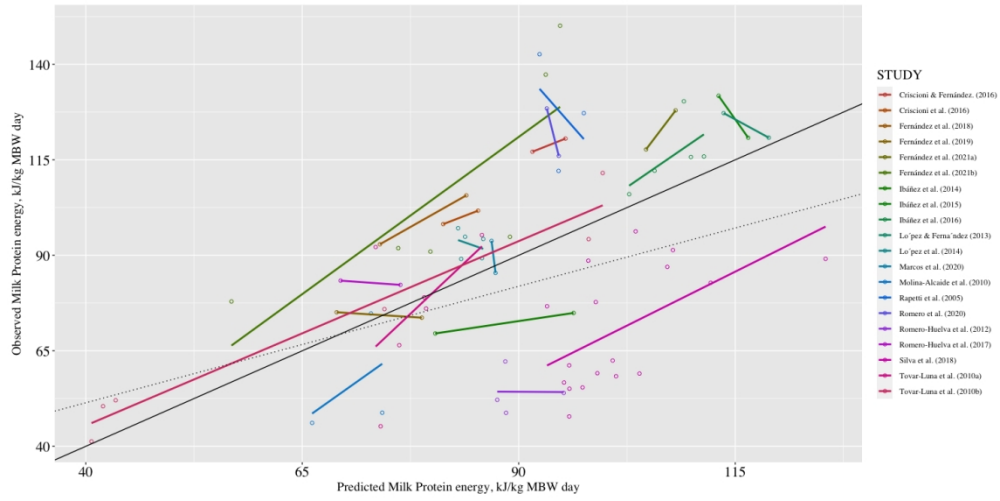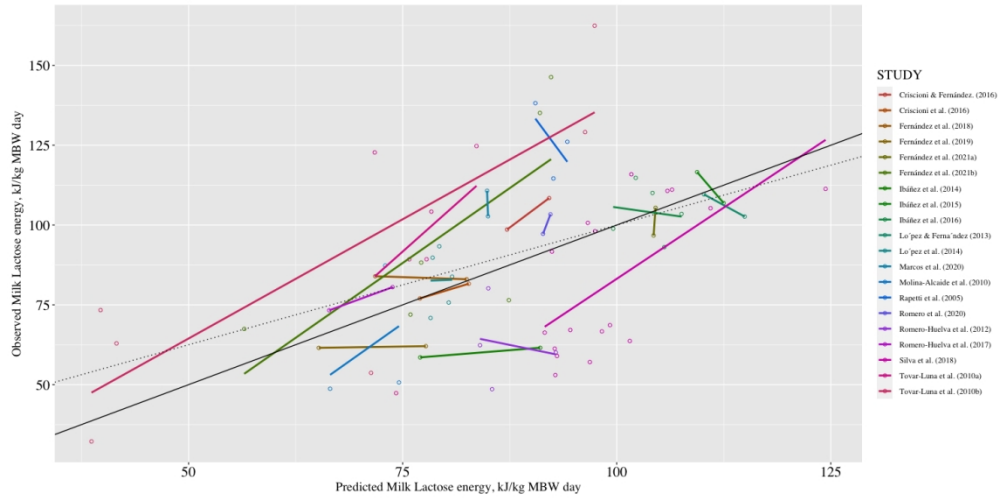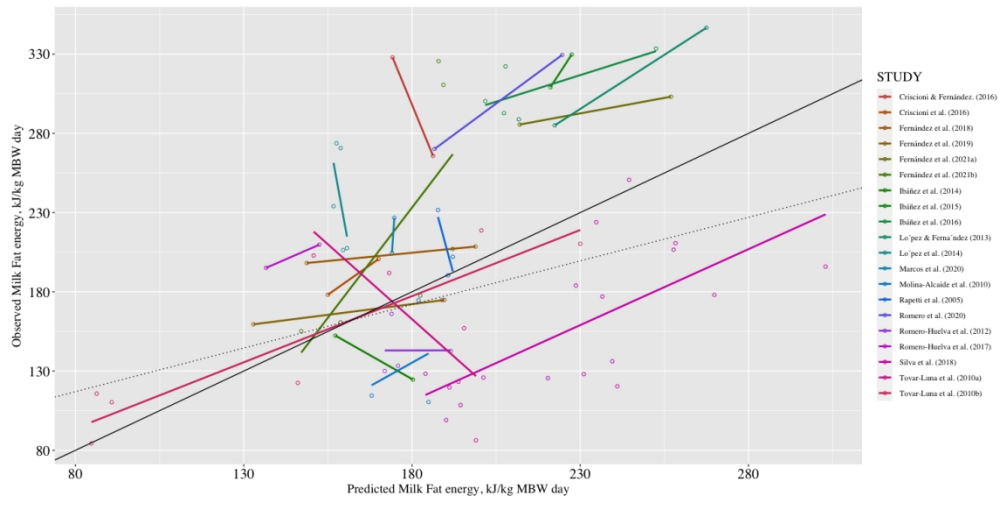252x181mm (72 x 72 DPI)
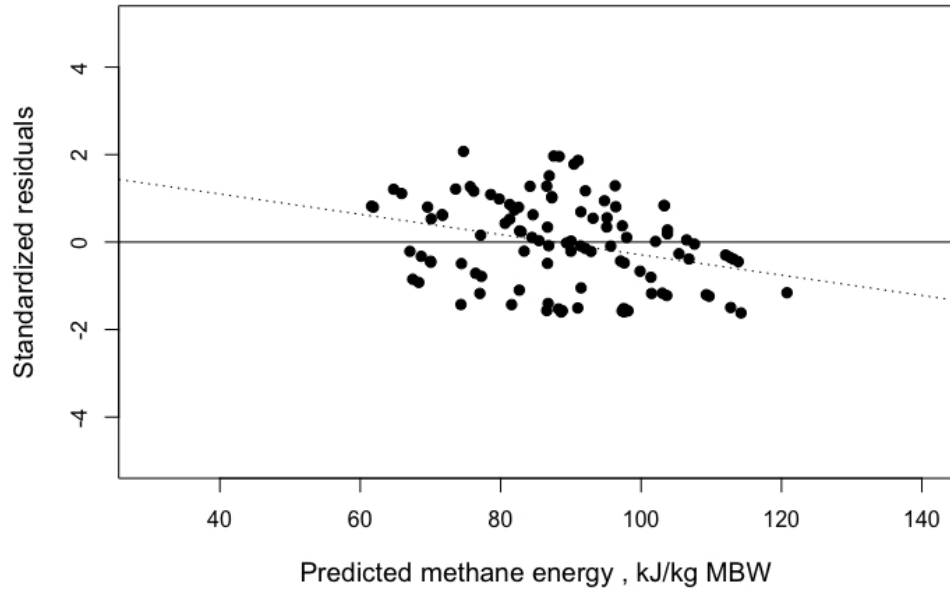
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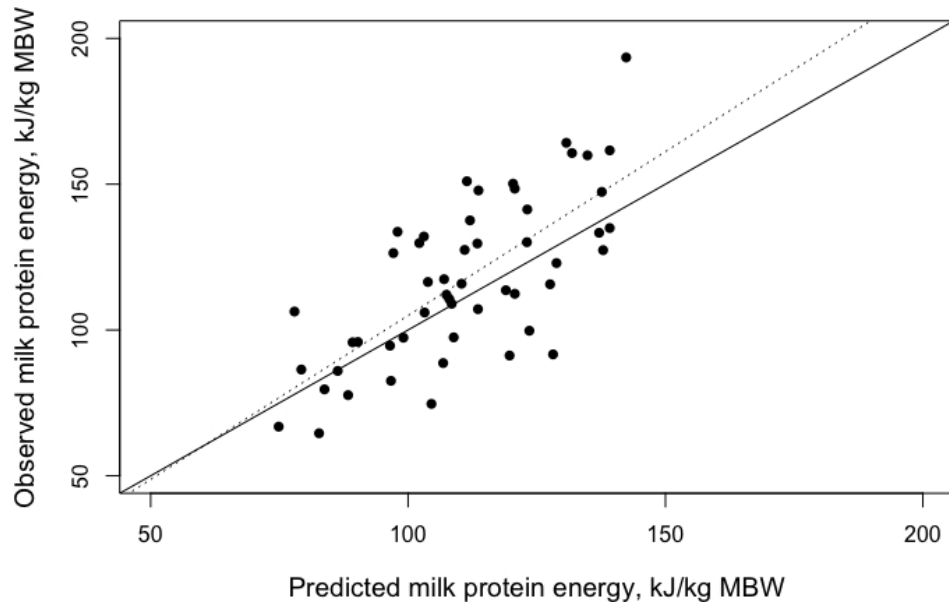
Figure 4. Observed versus predicted values of milk energy in protein (a), lactose (b) fat (c) and energy in methane (d) used for model internal evaluation in dairy goats [kJ/kg BW0.75 day; BW0.75 = MBW]. The regression equations were as follow: milk protein energy Y = -7.47 + 1.12X (standard error = 17.56 and 0.15 for the intercept and slope respectively; residual standard error = 19.83; R2 = 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; R2 = 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; R2 = 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; R2 = 0.43).

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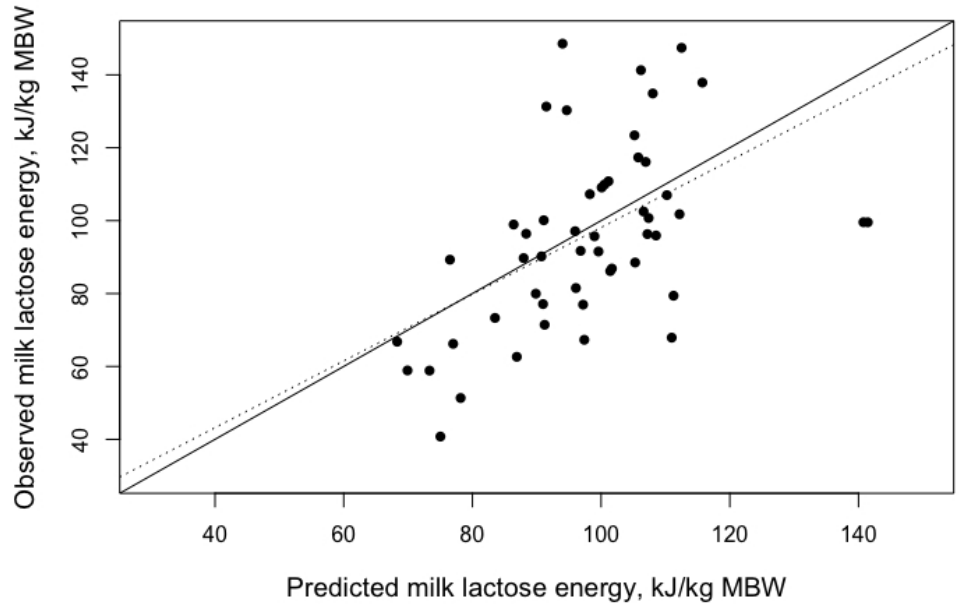
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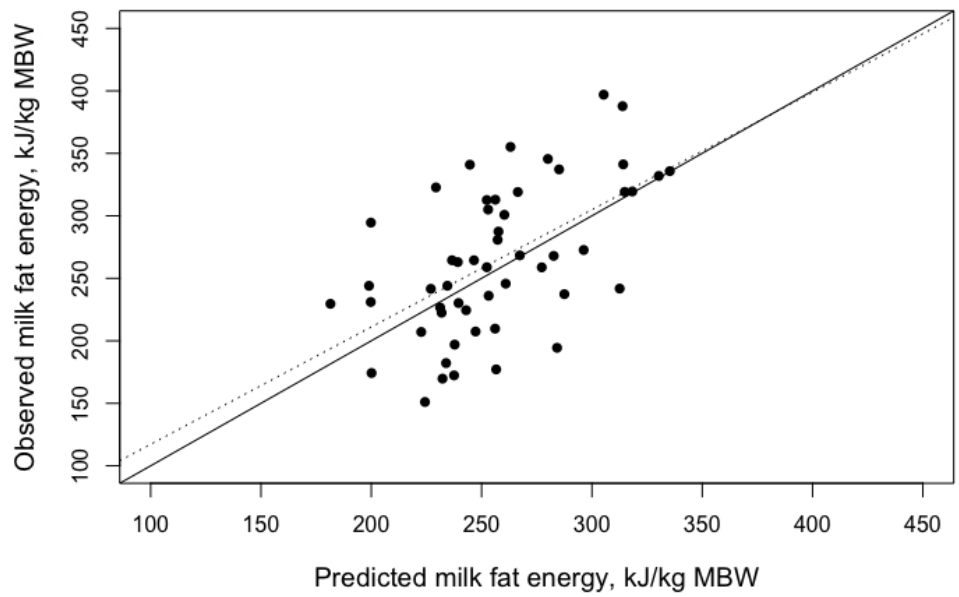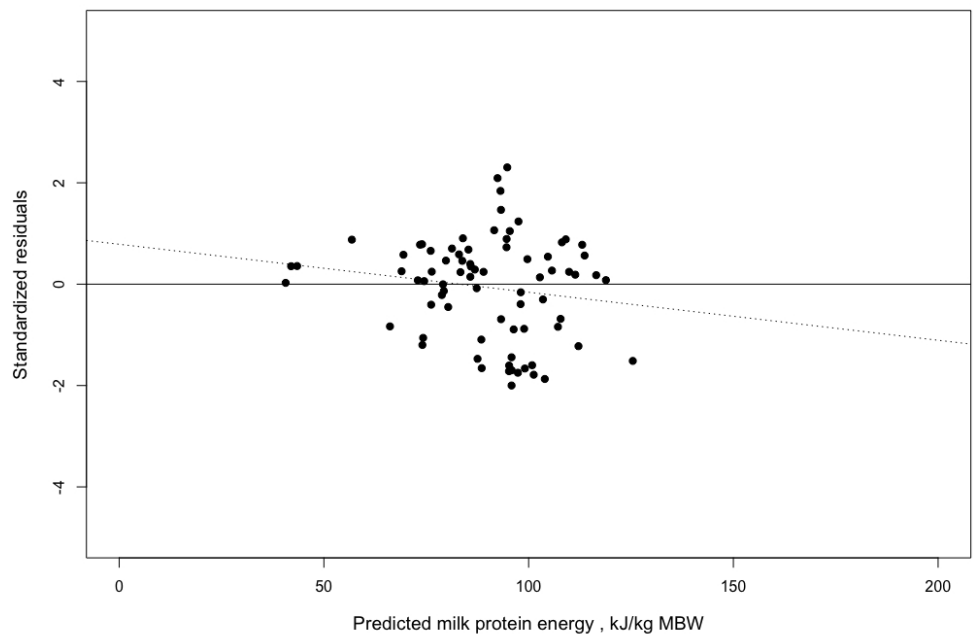
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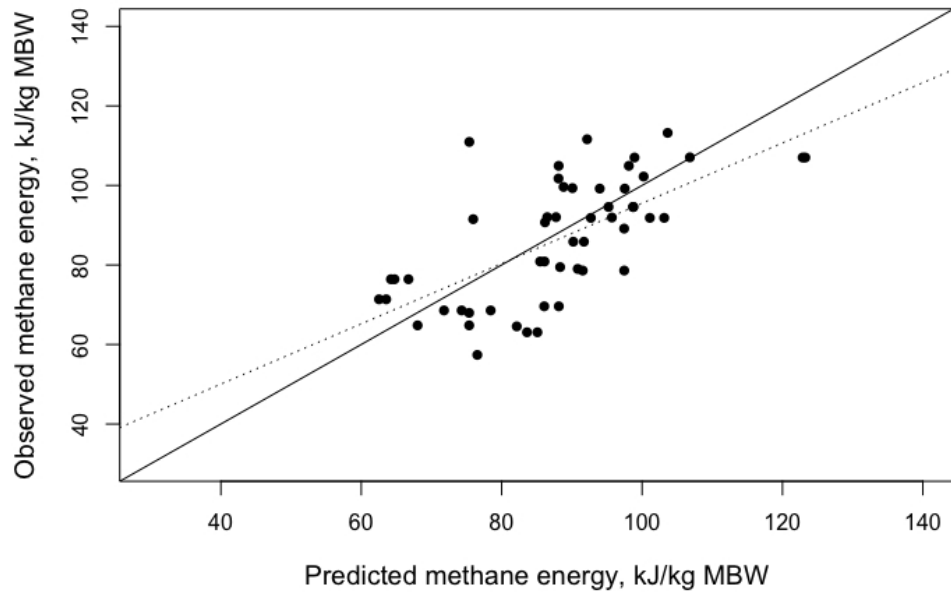
252x181mm (72 x 72 DPI)

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 BW0.75 day; BW0.75 = MBW].

252x181mm (72 x 72 DPI)

252x181mm (72 x 72 DPI)

252x181mm (72 x 72 DPI)

252x181mm (72 x 72 DPI)

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].

520x261mm (72 x 72 DPI)

520x261mm (72 x 72 DPI)
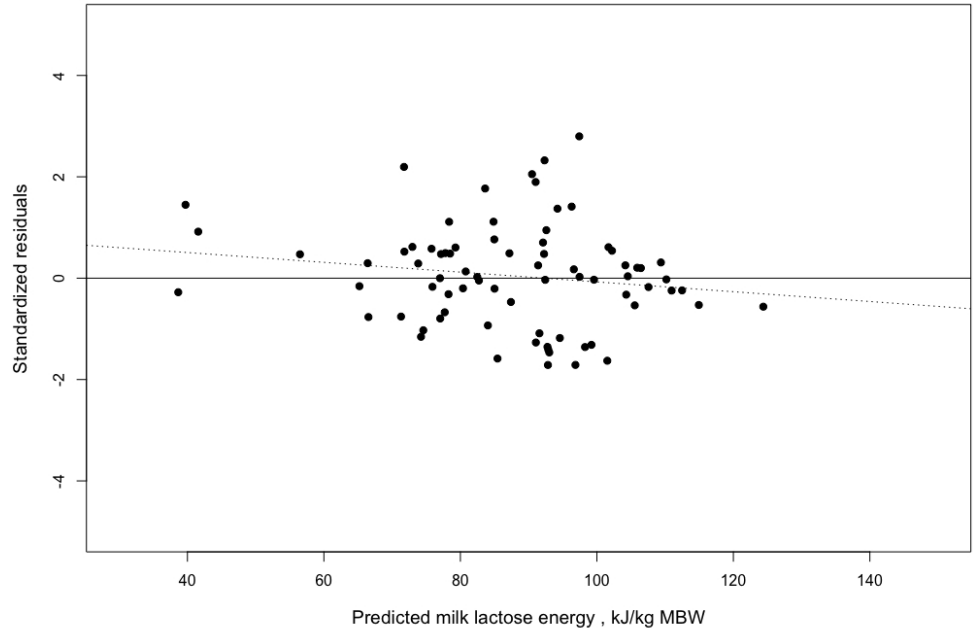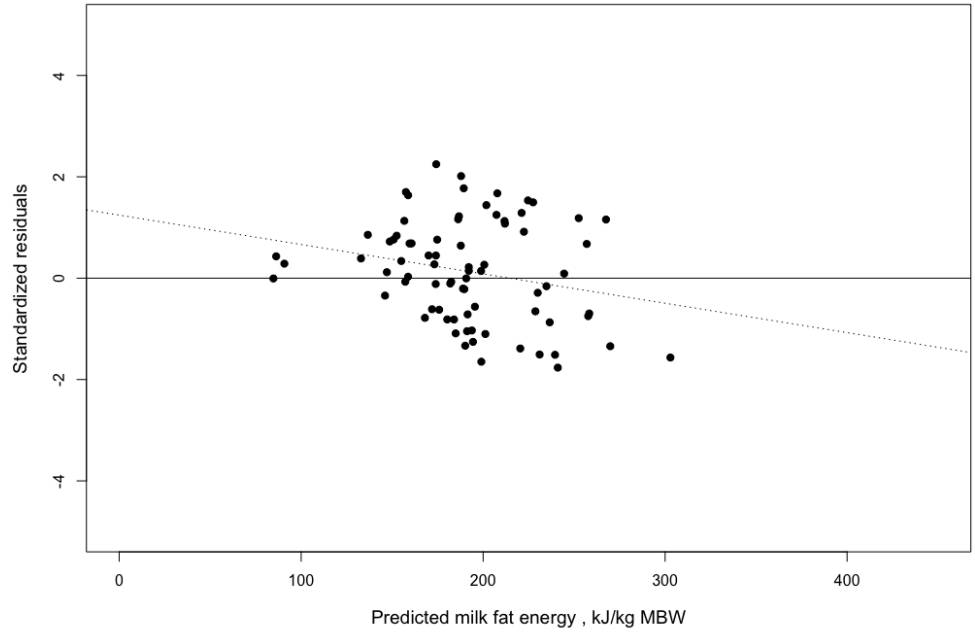
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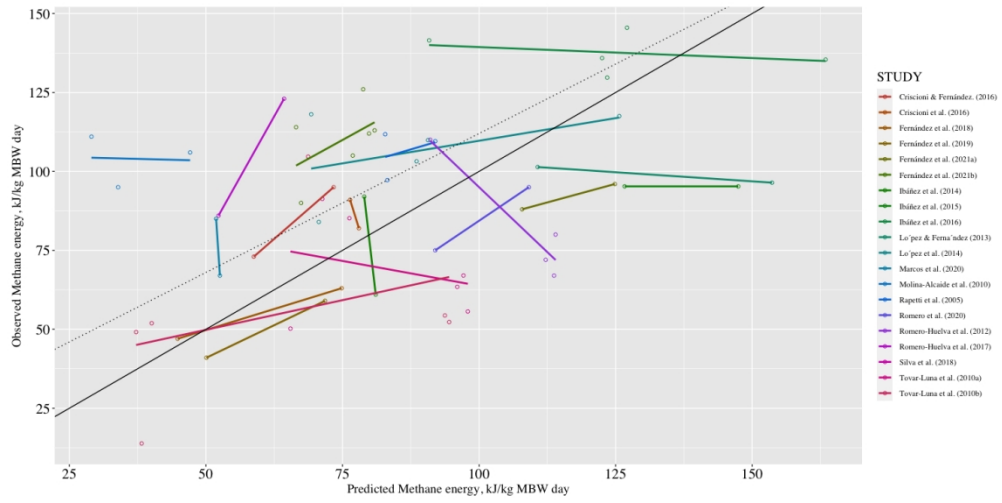
520x261mm (72 x 72 DPI)

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].
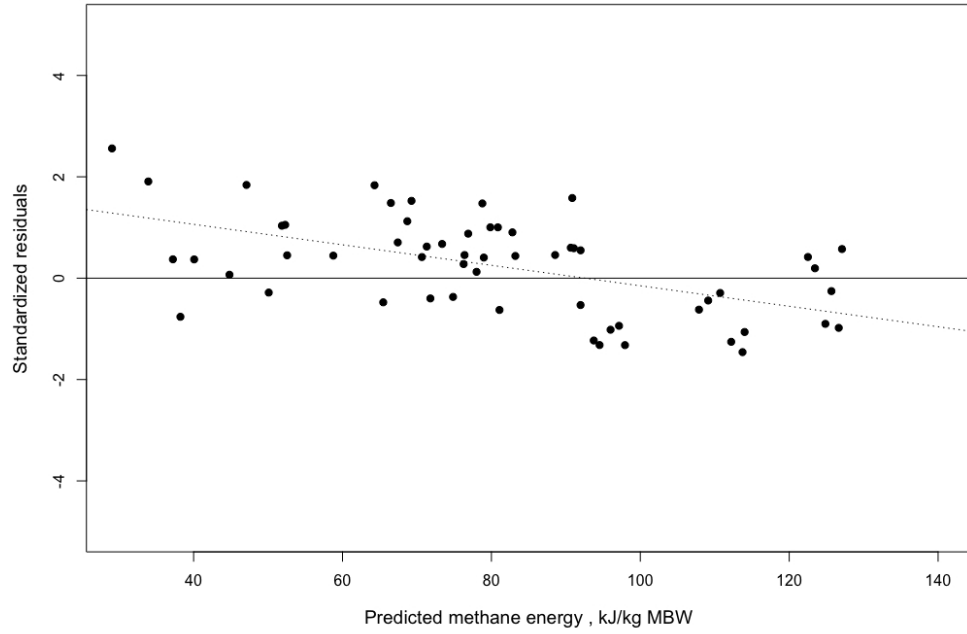
363x261mm (72 x 72 DPI)

363x261mm (72 x 72 DPI)

363x261mm (72 x 72 DPI)

363x261mm (72 x 72 DPI)