# SUPPLEMENT: EXPERIMENTAL AND COMPUTATIONAL DATA AND THERMODYNAMIC PROPERTIES

Experimental data adapted from Ladyman et al.\* included the incremental body weights for the first 7 days and the last day of the pregnancy. Empirically fitted cumulative incremental weight data curve (**Fig. S1**) was used to calculate the energy accumulation in the mass of the adipose tissue (*m1*) and in the mass of the uterus (*m2*) on a daily basis.

● Experimental data

Curve fitting

**Fig. S1.** Empirically fitted cumulative incremental weight data\*.

\*Ladyman SR., Carter KM, Grattan DR. (2018) Energy homeostasis and running wheel activity during pregnancy in the mouse. *Physiol Behav.* 194, 83-94. <https://doi.org/10.1016/j.physbeh.2018.05.002>.

Changes in the weights of the body, adipose tissue, offspring, placenta, amniotic fluid weights together with the chemical energy waste with feces, chemical energy accumulation in the abdominal fat and the chemical energy expense of the offspring and placenta are presented in **Table S1**. Oxidation reactions of major food components present in the control diet; their amounts (mg/g) and the moles of ATP produced by oxidation of 1 mole of component is presented in **Table S2**. Energy of entering into subsystem 3 with food was calculated by referring to energies of its major components (**Table S3**). Major fatty acid composition of the adipose tissue of the Sprague-Dawley pregnant rats is adapted from Kassem et al. (2012) and presented in**Table S4.** Specific constants of the elements employed to calculate the specific heats via Eq.3are presented in **Table S5.** Enthalpies of formation at 298.15 K were calculated either by group contribution method (Eq.1) or adapted the from NIST webbook (**Table S6**). Since all of the oxidation reactions of the food constituents took place in the body, their thermodynamic properties were calculated at 310 K with Eq.2. Molar chemical exergies of the system components are listed in **Table S7,** daily exergy waste with feces are listed in **Table S8.** Values of each term of Eq 16 were evaluated based on the experimental data. Uncertainty in these terms, including variability in the exergy of the nutrients due to variability in the amounts of food consumed, variability in the exergy of the faeces, due to variability in the excretion rates, etc., is presented in **Table S9,** including uncertaintyper unit exergy destroyed, *Exdest***.**

**Table S1.** Daily incremental changes in the weights of the total body of the mice and those of the adipose tissue, offspring, placenta and the amniotic fluid. The corresponding daily incremental chemical energy waste with feces, accumulation with abdominal fat and the chemical energy expense of the synthesis of the offspring and placenta are also presented here.

|  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Days** | **Body weight change (g)** | **Feces (g)** | **Adipose tissue weight increase (m1) (g)** | **Offspring weight increase (m2,1) (g)** | **Placenta weight increase (m2,2) (g)** | **Amniotic fluid weight increase (m2,3) (g)** | **Chemical energy waste with feces (kJ)** | **Chemical energy accumulation in abdominal fat (kJ)** | **Chemical energy expense of offspring (kJ)** | **Chemical energy expense of placenta (kJ)** |
| 2 | 23.6 | 1.76x10-3 | 4x10-2 | 7x10-2 | 5x10-2 | 7x10-2 | 0.3 | 0.1 | 0.3 | 1.24 |
| 3 | 23.5 | 1.94x10-3 | 1x10-2 | 1x10-2 | 1x10-2 | 1x10-2 | 0.4 | 2x10-2 | 5x10-2 | 0.2 |
| 4 | 23.6 | 2.02x10-3 | 1x10-2 | 2x10-2 | 1x10-2 | 2x10-2 | 0.4 | 4x10-2 | 0.1 | 0.4 |
| 5 | 23.8 | 2.04x10-3 | 1x10-2 | 2x10-2 | 1x10-2 | 2x10-2 | 0.4 | 4x10-2 | 0.1 | 0.4 |
| 6 | 24.3 | 2.17x10-3 | 5x10-2 | 7x10-2 | 5x10-2 | 8x10-2 | 0.4 | 0.1 | 0.3 | 1.4 |
| 7 | 24.9 | 2.16x10-3 | 1x10-1 | 2x10-2 | 0.1 | 0.16 | 0.4 | 0.3 | 0.6 | 2.8 |
| 8 | 25.6 | 2.20x10-3 | 2x10-1 | 3x10-2 | 0.2 | 0.31 | 0.4 | 0.5 | 1.2 | 5.4 |
| 9 | 26.6 | 1.94x10-3 | 2x10-1 | 3x10-2 | 0.2 | 0.29 | 0.4 | 0.5 | 1.1 | 5.1 |
| 10 | 27.7 | 2.12x10-3 | 2x10-1 | 3x10-2 | 0.2 | 0.35 | 0.4 | 0.5 | 1.3 | 6.0 |
| 11 | 29.0 | 2.35x10-3 | 3x10-1 | 4x10-2 | 0.3 | 0.40 | 0.4 | 0.6 | 1.5 | 6.9 |
| 12 | 30.4 | 2.29x10-3 | 3x10-1 | 4x10-2 | 0.3 | 0.45 | 0.4 | 0.7 | 1.7 | 7.9 |
| 13 | 32.1 | 2.47x10-3 | 3x10-1 | 5x10-2 | 0.3 | 0.51 | 0.5 | 0.8 | 1.9 | 8.8 |
| 14 | 33.9 | 2.87x10-3 | 3x10-1 | 5x10-2 | 0.4 | 0.56 | 0.5 | 0.9 | 2.1 | 9.7 |
| 15 | 35.8 | 2.71x10-3 | 4x10-1 | 6x10-2 | 0.4 | 0.61 | 0.5 | 1.0 | 2.3 | 10.6 |
| 16 | 38.0 | 2.92x10-3 | 4x10-1 | 6x10-2 | 0.4 | 0.67 | 0.5 | 1.0 | 2.5 | 11.6 |
| 17 | 40.3 | 2.94x10-3 | 4x10-1 | 7x10-2 | 0.5 | 0.72 | 0.6 | 1.1 | 2.7 | 12.5 |
| 18 | 42.7 | 2.81x10-3 | 5x10-1 | 7x10-2 | 0.5 | 0.77 | 0.5 | 1.2 | 2.9 | 13.4 |

**Table S2.** Oxidation reactions of major food components present in the control diet; their amounts (mg/g) and the moles of ATP produced by oxidation of 1 mole of component

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
|  | **Food Components** | **mg /g diet** | **Oxidation Reactions** | **ATP (mole)** |
| Fat part | Linoleic acid (C18:2) | 28.5 | C18H32O2 + 25 O2 →18 CO2 + 16 H2O | 146 a |
| Oleic acid | 13.5 | C18H34O2 + 51/2 O2 → 18 CO2 + 17 H2O | 146 a |
| Palmitic acid | 2.5 | C16H32O2 + 23 O2 → 16 CO2 + 16 H2O | 129 a |
| Stearic acid | 1.4 | C18H36O2+ 26 O2 → 18 CO2 + 18 H2O | 146 b |
| Alpha-Linolenic acid (C18:3) | 0.2 | C18H30O2 + 49/2 O2 → 18 CO2 + 15 H2O | 146 a |
| Arachidic acid (C20:0) | 0.1 | C20H40O2 + 29 O2 → 20 CO2 + 20 H2O | 163 a |
| Eicosenoic acid (C20:1) | 0.2 | C20H38O2 + 57/2 O2 → 20 CO2 + 19 H2O | 163 a |
| Carb. Part | Polysaccharides (Starch) | 471.7 | C6H12O6 + 6 O2 → 6 CO2 + 6 H2O | 38 a |
| Disaccharide (Sucrose) | 98.1 | C12H22O11 + H2O→ C6H12O6 + C6H12O6  Glucose Fructose | 38 a,\*  39 a,\*\* |

a Calculated according to the catabolic pathways

b Guyton AC & Hall JE. (2016). Guyton and Hall Textbook of medical physiology (13th edition), USA: Elsevier.

**\*** ATP produced from one mole from glucose; \*\*from one mole of fructose

**Table S3.** Contribution of the food and oxygen intake and carbon dioxide production and ΔHrxn of the metabolism of the food components in oxidation reactions

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Days** | **Total Food Intake (g)** | **Entering Food Amount to Subsystem 3 (g)** | **Energy Entering with Food to Subsystem 3 (kJ) #** | **Energy of the inhaled oxygen (kJ)** | | **Energy of the exhaled the carbon dioxide (kJ) #** | **Energy of the metabolically produced leaving water (kJ) #** | ***ΔHrxn* (kJ) #**  **(*Σn Δhf, products* – *Σm Δhf, reactant*)** | ***ΔHrxn* (kJ) in their absolute valueafter multiplied with RER values** |
| 2 | 2.6 | 2.1 | -8.6 | 1.7x10-2 | -18.0 | | -10.9 | -20.3 | 18.2 |
| 3 | 2.9 | 2.5 | -10.3 | 2.1x10-2 | -21.6 | | -13.1 | -24.2 | 22.0 |
| 4 | 3.0 | 2.6 | -10.6 | 2.1x10-2 | -22.2 | | -13.5 | -25.1 | 22.7 |
| 5 | 3.0 | 2.6 | -10.8 | 2.2x10-2 | -22.5 | | -13.7 | -25.5 | 23.0 |
| 6 | 3.2 | 2.6 | -10.7 | 2.2x10-2 | -22.4 | | -13.6 | -25.4 | 22.9 |
| 7 | 3.2 | 2.3 | -9.6 | 1.9x10-2 | -20.0 | | -12.2 | -22.6 | 20.8 |
| 8 | 3.3 | 1.9 | -7.8 | 1.6x10-2 | -16.3 | | -9.9 | -18.4 | 16.9 |
| 9 | 2.9 | 1.6 | -6.6 | 1.3x10-2 | -13.8 | | -8.3 | -15.6 | 14.3 |
| 10 | 3.1 | 1.7 | -6.9 | 1.4x10-2 | -14.3 | | -8.7 | -16.2 | 15.1 |
| 11 | 3.5 | 1.8 | -7.4 | 1.5x10-2 | -15.5 | | -9.4 | -17.5 | 16.3 |
| 12 | 3.4 | 1.5 | -6.3 | 1.3x10-2 | -13.3 | | -8.1 | -15.0 | 14.0 |
| 13 | 3.7 | 1.6 | -6.6 | 1.3x10-2 | -13.8 | | -8.4 | -15.6 | 15.0 |
| 14 | 4.2 | 1.9 | -8.0 | 1.6x10-2 | -16.8 | | -10.2 | -19.0 | 18.3 |
| 15 | 4.0 | 1.6 | -6.5 | 1.3x10-2 | -13.6 | | -8.3 | -15.4 | 14.8 |
| 16 | 4.3 | 1.7 | -6.9 | 1.4x10-2 | -14.5 | | -8.8 | -16.3 | 15.7 |
| 17 | 4.4 | 1.5 | -6.3 | 1.3x10-2 | -13.3 | | -8.1 | -15.0 | 14.4 |
| 18 | 4.2 | 1.2 | -4.9 | 9.9x10-2 | -10.3 | | -6.3 | -11.7 | 11.2 |

#The negative sign, which comes from the standard enthalpy of formation of the components, was used in the calculations of the *ΔHrxn*. In the energy balance, absolute values of the *ΔHrxn* were used

### **Table S4.** Major fatty acid composition of the adipose tissue of the Sprague-Dawley pregnant rats (adapted from Kassem et al., 2012\*)

|  |  |
| --- | --- |
| **Major fatty acids** | **% Composition of abdominal fat** |
| oleic acid | 35.6% |
| linoleic acid | 31.9% |
| palmitic acid | 20.8% |
| stearic acid | 4.0% |
| palmitoleic acid | 2.2% |

**\*** Kassem AA, Bakar A, Zuki M, Yong Meng G, Mustapha NM. (2012) Dietary (n-6: n-3) fatty acids alter plasma and tissue fatty acid composition in pregnant Sprague Dawley rats. *Sci. World J.* 851437.

**Table S5.** Specific constants of elements employed while calculating the specific heats with Eq.3 (adapted from Hurst and Harrison, 1992\*)

|  |  |  |
| --- | --- | --- |
| **Atom** | **Specific constant (cE) for liquids** | **Specific constant (cE) for solids** |
| H | 9.20 | 7.56 |
| C | 13.08 | 10.89 |
| O | 16.00 | 13.42 |
| N | 30.19 | 18.74 |
| S | 32.05 | 12.36 |

**\*** Hurst Jr, JE & Keith Harrison B. (1992) Estimation of liquid and solid heat capacities using a modified Kopp's rule. Chem. Eng. Commun. 112(1); 21-30

**Table S6.** Molecular weight, MW, specific heat and the enthalpy of formation of the major components of the diet

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| **Chemical Components** |  | **MW**  **(g/mol) a** | ***cp, 298.15K* (kJ/mol K)** | ***Δh°f, 298.15K* (kJ/mol)** | ***Δh°f, 310.15 K* (kJ/mol) h** |
| Linoleic acid (C18:2) |  | 280.5 | 0.56 d,\* | -634.7 a,\* | -628.0 |
| Oleic acid |  | 282.5 | 0.58 e,\* | -764.8 a,\* | -757.9 |
| Palmitic acid |  | 256.4 | 0.54 d,\* | -848.4 a,\* | -842.0 |
| Stearic acid |  | 284.5 | 0.58 d,\* | -912.0 a,\* | -905.0 |
| Alpha-Linolenic acid (C18:3) |  | 278.4 | 0.55 d,\* | -508.8 a,\* | -502.2 |
| Arachidic acid (C20:0) |  | 312.5 | 0.66 d,\* | -806.4 b,\* | -798.5 |
| Eicosenoic acid (C20:1) |  | 310.5 | 0.65 d,\* | -689.4 b,\* | -681.6 |
| Palmitoleic acid |  | 254.4 | 0.52 d,\* | -713.4 a,\* | -707.1 |
| Polysaccharides (Starch) |  | 180.2 | 0.22 a | -1267.1 c | -1264.5 |
| Disaccharide (Sucrose) | Glucose | 180.2 | 0.22 a | -1267.1 c | -1264.5 |
| Fructose | 180.2 | 0.23 g | -1265.2 a | -1262.5 |
| Oxygen |  | 32.0 | 0.03 f,\*\* | 0.00 a,\*\* | 0.4 |
| Carbon dioxide |  | 44.0 | 0.04 f,\*\* | -393.5 a,\*\* | -393.1 |
| Water |  | 18.0 | 0.03 f,\*\* | -241.8 a,\*\* | -241.4 |

\* refers liquid, \*\* refers gaseous state and the others are at solid-state

Negative ∆h°f values mean that formation reactions are exothermic

a Afeefy HY, Liebman JF, Stein SE. (2018) “Neutral Thermochemical Data” in NIST Chemistry Webbook, NIST Standard Reference Database No. 69, Linstrom, P. J., Mallard, W. G. (Eds). National Institute of Standards and Technology, Gaithersburg MD

b Calculated by group contribution method

c Hammes GG, Hammes-Schiffer S. (2015) Physical chemistry for the biological sciences. New Jersey: John Wiley & Sons.

d Calculated by Eq.3

e Lide DR. (2004) CRC handbook of chemistry and physics (Vol. 85). CRC press.

f Öztürk A, Kılış A, Yavuz H. (2007) Termodinamik ve Isı Geçişi Tabloları (4th edition). Istanbul: Çağlayan Kitapevi:12.

g Kawaizumi F, Nishio N, Nomura H, Miyahara Y. (1981) Heat-capacity measurements of aqueous solutions of mono-, di-, and tri-saccharides using an isoperibol twin calorimeter. J. Chem. Thermodyn.; 13(1); 89–98.

h Calculated by Eq.2

**Table S7.** Molar chemical exergies of the system components at 310.15 K

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Chemical Components** |  | | ***Δg°f, 310.15 K* (kJ/mol)** | | | ***ex°chem*, 310.15 K (kJ/mol)** |
| Linoleic acid (C18:2) |  | | -60.3 | | | 11105.8 |
| Oleic acid |  | | -138.5 | | | 11263.7 |
| Palmitic acid |  | | -112.6 | | | 10232.9 |
| Stearic acid |  | | -216.0 | | | 11422.3 |
| Alpha-Linolenic acid (C18:3) |  | | 14.2 | | | 10944.2 |
| Arachidic acid (C20:0) |  | | -202.7 | | | 12728.2 |
| Eicosanoid acid (C20:1) |  | | -130.2 | | | 12564.7 |
| Palmitoleic acid |  | | -121.9 | | | 9954.4 |
| Polysaccharides (Starch) |  | | -896.3 | | | 2985.8 |
| Disaccharide (Sucrose) | Glucose | | -896.3 | | | 2985.8 |
| Fructose | | | -967.3 | | 2922.7 |
| Oxygen |  | | | | 0.0 | 4.0 |
| Carbon dioxide | |  | -394.4 | | | 19.8 |
| Water (gaseous) |  | | -228.0 | | | 10.1 |

*Δg°f, 310.15 K* values were calculated by Eq.14 *ex°chem*, 310.15 K values were calculated by Eq.15

**Table S8.** Exergy wasted with feces and exergy expense of the adipose tissue, offspring and the placenta

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Days** | **Exergy waste with feces (kJ)** | **Exergy accumulation in abdominal fat (kJ)** | **Exergy expense to the offspring (kJ)** | **Exergy expense of the placenta (kJ)** |
| 2 | 0.83 | 1.66 | 0.23 | 1.04 |
| 3 | 0.91 | 0.32 | 0.04 | 0.20 |
| 4 | 0.95 | 0.52 | 0.07 | 0.33 |
| 5 | 0.96 | 0.52 | 0.07 | 0.33 |
| 6 | 1.02 | 1.81 | 0.25 | 1.14 |
| 7 | 1.02 | 3.69 | 0.50 | 2.32 |
| 8 | 1.03 | 7.16 | 0.98 | 4.50 |
| 9 | 0.91 | 6.80 | 0.93 | 4.28 |
| 10 | 1.00 | 8.03 | 1.10 | 5.05 |
| 11 | 1.11 | 9.26 | 1.26 | 5.83 |
| 12 | 1.08 | 10.49 | 1.43 | 6.60 |
| 13 | 1.16 | 11.73 | 1.60 | 7.37 |
| 14 | 1.35 | 12.96 | 1.77 | 8.15 |
| 15 | 1.27 | 14.19 | 1.94 | 8.92 |
| 16 | 1.37 | 15.42 | 2.10 | 9.69 |
| 17 | 1.38 | 16.65 | 2.27 | 10.47 |
| 18 | 1.32 | 17.88 | 2.44 | 11.24 |

**Table S9.** Estimated uncertainties of exergy balance components and calculated uncertainty of Exdest

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **Estimated uncertainties in the components of the exergy balance (kJ)** | | | | **Estimated uncertainty in exergy destroyed (kJ)** |
| **Days** |  |  |  |  |  |
| 2 | 1.1 | 0.1 | 0.03 | 0.4 | 1.6 |
| 3 | 1.3 | 0.1 | 0.03 | 0.5 | 1.9 |
| 4 | 1.3 | 0.1 | 0.03 | 0.5 | 2.0 |
| 5 | 1.3 | 0.1 | 0.03 | 0.6 | 2.0 |
| 6 | 1.3 | 0.1 | 0.03 | 0.5 | 2.0 |
| 7 | 1.2 | 0.1 | 0.03 | 0.5 | 1.8 |
| 8 | 1.0 | 0.1 | 0.02 | 0.4 | 1.5 |
| 9 | 0.8 | 0.1 | 0.02 | 0.3 | 1.3 |
| 10 | 0.9 | 0.1 | 0.02 | 0.4 | 1.3 |
| 11 | 1.0 | 0.1 | 0.02 | 0.4 | 1.4 |
| 12 | 0.8 | 0.1 | 0.02 | 0.3 | 1.2 |
| 13 | 0.9 | 0.1 | 0.02 | 0.4 | 1.3 |
| 14 | 1.1 | 0.1 | 0.03 | 0.5 | 1.6 |
| 15 | 0.9 | 0.1 | 0.02 | 0.4 | 1.3 |
| 16 | 0.9 | 0.1 | 0.02 | 0.4 | 1.4 |
| 17 | 0.8 | 0.1 | 0.02 | 0.4 | 1.3 |
| 18 | 0.7 | 0.1 | 0.02 | 0.3 | 1.0 |

The assumed uncertainties are 5, 7, 10 and 10% for exergy input, exergy output, heat exergy and work fluxes, respectively. Calculations are based on the procedure described in “A Summary of Error Propagation”; Physical Sciences, Harvard University, Fall 2011; available at [*http://ipl.physics.harvard.edu/wp-uploads/2013/03/PS3\_Error\_Propagation\_sp13.pdf*](http://ipl.physics.harvard.edu/wp-uploads/2013/03/PS3_Error_Propagation_sp13.pdf)