MODELING HEAT PRODUCTION BY AOX PATHWAY IN SINGLE CELL

Assumptions

1. The non-growth rate of ATP production is 7.6 mmol per gram of biomass per hour (Ecoli W3110) at 38C. This rate is slightly higher in growth-associated conditions (13 mmol/g/h). (Varma & Palsson, 1994)

2. AOX branches from the cytochrome pathway at the level of the ubiquinone pool and couples the oxidation of ubiquinol to the four-electron reduction of oxygen to water. (Albury, Elliott & Moore, 2009)

3. Electrochemical potential gradient difference between Uq and O2 is 800 mV (Ingledew & Poole, 1984)

4. Two electrons are required per production of 1 ATP molecule

5. The dry mass of one E. coli cell = 7*10^-13 g (http://bionumbers.hms.harvard.edu/bionumber.aspx?s=y&id=103904&ver=9)

Calculations

The amount of energy released by 4 electrons is given by:

$$Volt = \frac{Joule}{Coulomb} \Rightarrow$$

$$800 \times 10^{-3} = \frac{Joules}{(4\ electrons)(1.6 \times 10^{-19}\ C)}$$

$$Energy\ released = 5.12 \times 10^{-19}\ Joules$$

The amount of energy per cell per second is given by:

$$\frac{7.6 \times 10^{-3}\ mol\ ATP}{3600\ sec \times g.\ biomass} \times \frac{2\ mol\ elec}{mole\ ATP} \times \frac{6.0223 \times 10^{23}\ electrons}{mol\ elec} \times \left(\frac{5.12 \times 10^{-19}\ J}{4\ electrons}\right) \times 0.7$$

$$= 0.2278\ \frac{J}{g\ biomass \times sec} = 1.6 \times 10^{-13}\ \frac{J}{cell \times sec}$$

(where 0.7 is an efficiency factor representing approximately 70% conversion of electrons in the pathway in sacred lotus cells [Applied and Environmental Microbiology, Oct. 1994, p. 3724-3731 Vol 60 No 10])

By way of comparison, the specific heat of water is 4.187 J per ml (when 1 ml = 1 gram).

Characterization methods

There are currently a few possible ways to characterize the heat production that largely break down into two categories: measuring in saturated bulk solution, and measuring colonies on a plate.

Measuring in saturated bulk solution:

Measuring in bulk means heating up solution and measuring either with sensitive thermometers or isothermal calorimetry. Taking a saturated 1 ml sample in solution would take an inordinate amount of time to see even a 1 C rise:

$$1\ \text{ml} \times 1\times10^{10}\ \frac{\text{cells}}{\text{ml}} \times 1.6\times10^{-13}\ \frac{\text{J}}{\text{cell}\times\text{sec}} = 1.6\times10^{-4}\ \frac{\text{J}}{\text{sec}}$$

$$4.187\ \frac{\text{J}}{\text{ml}} \times \frac{\text{seconds}}{1.6\times10^{-4}\ \text{J}} = 2{,}417\ \text{seconds} \times \frac{1\ \text{min}}{60\ \text{sec}} = 40.3\ \text{minutes}$$

Methods such as isothermal calorimetry have very precise detection ranges on the order of several microcal/sec that could possibly determine a temperature shift that happens in the timeframe of minutes instead of hours.

Measuring in colonies:

There are several types of thermal imaging that could possibly detect heat from colonies on a plate with a precision of approximately 0.1 C.