## Creatine kinase

Van Beek’s model[[1]](#footnote-20) for both mitochondrial IMS and cytosolic compartments.

Parameters were optimized by Hettling’s work.[[2]](#footnote-21)

ATP + Cr = ADP + PCr

### Mitochondrial CK (miCK)

| Parameter | Value | Unit | Desc. |
| --- | --- | --- | --- |
|  | 151.95 | - | Equilibrium constant for Cr production |
|  | 0.77505 | mM \* Hz | Maximum velocity for PCr production |
|  |  | mM \* Hz | Maximum velocity for Cr production |
|  | 0.75132 | mM | Binary dissociation constant for ATP |
|  | 5.20908 | mM | Ternary dissociation constant Cr |
|  | 0.20173 | mM | Binary dissociation constant ADP |
|  | 0.49951 | mM | Ternary dissociation constant PCr |
|  | 28.73344 | mM | Binary dissociation constant Cr |
|  | 1.59769 | mM | Binary dissociation constant PCr |
|  |  | mM | Ternary dissociation constant ADP |
|  |  | mM | Inhibition constant Cr |

### Cytosolic CK (mmCK)

| Parameter | Value | Unit | Desc. |
| --- | --- | --- | --- |
|  | 151.95 | - | Equilibrium constant for Cr production |
|  | 7.37307 | mM \* Hz | Maximum velocity for PCr production |
|  |  | mM \* Hz | Maximum velocity for Cr production |
|  | 1.2624 | mM | Binary dissociation constant for ATP |
|  | 16.74444 | mM | Ternary dissociation constant Cr |
|  | 0.21226 | mM | Binary dissociation constant ADP |
|  | 1.66976 | mM | Ternary dissociation constant PCr |
|  | 34.50419 | mM | Binary dissociation constant Cr |
|  | 4.51655 | mM | Binary dissociation constant PCr |
|  |  | mM | Ternary dissociation constant ADP |
|  |  | mM | Inhibition constant Cr |

## Creatine shuttle

Positive direction is from IMS to cytosol.

Since the diffusion rate is the same for ATP/ADP pair, and Cr/PCr pair, respectively. We can deduce more conservation relationships.

| Parameter | Value | Unit | Desc. |
| --- | --- | --- | --- |
|  | 23.64 | Hz | conductance of ATP |
|  |  | Hz | conductance of ADP |
|  | 155 | Hz | conductance of PCr |
|  |  | Hz | conductance of Cr |
|  | 195.63 | Hz | conductance Pi |
|  | 3 | - | Relative volume of cytosol. Volume of 1 corresponds to =0.153mL/gww. |
|  | 1 | - | Relative volume of mitochondrial matrix. |
|  | 0.25 | - | Relative volume of intermembrane space. |
|  | 5.665 | mM | Sum of cytosolic adenylate |
|  | 5.665 | mM | Sum of intermembrane space adenylate |
|  | 15.5 | mM | Pool of cytosolic creatine |
|  | 15.5 | mM | Pool of intermembrane space creatine |

## ODEs for High-energy and inorganic phosphates

1. Kongas O, van Beek JHGM Creatine kinase in energy metabolic signaling in muscle Nature Precedings (2007)DOI: https://doi.org/10.1038/npre.2007.1317.1 [↑](#footnote-ref-20)
2. Hettling, H., & van Beek, J. H. G. M. (2011). Analyzing the functional properties of the creatine kinase system with multiscale “sloppy” modeling. PLoS Computational Biology, 7(8), e1002130. [↑](#footnote-ref-21)