

**Correction to “Dynamic Simulations of Single Molecule Enzyme Networks”** [*The Journal of Physical Chemistry B* **2009**, *113*, 5537–5544. DOI: 10.1021/jp807520f]. Dieter Armbruster,\* John D. Nagy, E. A. F. van de Rijt, and J. E. Rooda

The original article showed the influence of the variance of the  $\Gamma$ -distribution for  $\tau_r$  on the cycle time and steady state concentrations of the initial steps (the Embden–Meyerhof–Parnas (EMP) steps) of glycolysis. Unfortunately, due to a coding error, the coefficient of variation  $c_v$  was between 30 and 120, instead of the value  $c_v = 3$  as claimed. Obviously, that amount of stochasticity is far too high for a biological system.

This does not affect the fundamental thesis of the paper that single molecule enzyme networks can easily be simulated in a much more flexible way through discrete event simulations than through the traditional Gillespie algorithm. However, it does influence the *quantitative results* of the EMP steps of glycolysis used as an example and reported in the article.

Specifically, the stable regime of glycolysis is limited by an approximate 2:1 ratio of the mean interarrival time of glucose molecules  $t_a$  and the mean conversion time  $t_c$  from ADP back to ATP. The stochasticity of the processes changes that ratio slightly to  $t_c/t_a \geq \approx 0.48$  but not, as previously reported to  $t_c/t_a \geq \approx 0.40$ . To determine the influence of the stochasticity for  $c_v = 3$ , we repeated the simulations for the marginally stable (most susceptible to stochastic variations) case of  $t_a = 0.025$  and  $t_c = 0.012$  and report them in Table 1. More details can be found in ref 1 (section 6).

**Table 1. Comparison between Simulations of the EMP Steps of Glycolysis at Steady State<sup>a</sup>**

	Gluc	CV	G6P	CV	F6P	CV	ATP	CV	ADP	CV
det	55.00		26.00		214.00		198.48		0.31	
stoch	63.48	0.20	26.05	0.19	217.24	0.05	180.19	0.10	18.56	0.93
diff (%)	15.41		0.19		1.52		−9.22		5830.22	

<sup>a</sup>We list the mean equilibrium levels for glucose, G6P, F6P, ATP, and ADP for a simulation based on deterministic processing rates and stochastic simulations based on exponential search time distributions and  $\Gamma$ -distributed reconfiguration times. The coefficients of variation for the stochastic simulations are also shown.

## REFERENCES

(1) van Zwieten, D. A. J.; Rooda, J. E.; Armbruster, D.; Nagy, J. D. *Discrete event simulations for glycolysis pathway and energy balance*; SE Report 2010-02; Eindhoven University of Technology: Eindhoven, The Netherlands, 2010; <http://se.wtb.tue.nl/sereports>.

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