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Dynamics and thermodynamics of open chemical networks MASSIMILIANO ESPOSITO, University of Luxembourg — Open chemical networks (OCN) are large sets of coupled chemical reactions where some of the species are chemostated (i.e. continuously restored from the environment). Cell metabolism is a notable example of OCN. Two results will be presented. First, dissipation in OCN operating in nonequilibrium steady-states strongly depends on the network topology (algebraic properties of the stoichiometric matrix) [1]. An application to oligosaccharides exchange dynamics performed by so-called D-enzymes will be provided [2]. Second, at low concentration the dissipation of OCN is in general inaccurately predicted by deterministic dynamics (i.e. nonlinear rate equations for the species concentrations). In this case a description in terms of the chemical master equation is necessary. A notable exception is provided by so-called deficiency zero networks, i.e. chemical networks with no hidden cycles present in the graph of reactant complexes [3].

[1]M. Polettini and M. Esposito, J. Chem. Phys. 141, 024117 (2014)
[2]R. Rao, D. Lacoste and M. Esposito, arxiv:1509.07446
[3]M. Polettini, A. Wachtel and M. Esposito, arxiv:1507.00058

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