Structural improvement of dynamic flux balance analysis for speeding up the simulation

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A kinetic model which has several lower optimization steps in its structure and employs an optimized objective value can be considered as a special case of bi-level optimization problem when it is implemented by an upper level optimization such as a parameter estimation. But this kind of modeling is not free from a computational load issue because of its double layered optimizing structure. So, in order to overcome this limitation, this paper suggests a method by which the embedded lower level linear optimization problem is solved before the result is employed to modeling. In other words, the linear optimization is solved with remaining an undetermined variable k coming from other equations in modeling. And the optimized objective value is expressed as a function of k, then finally the result is employed for upper level optimization. In this way, its structure is no more the double layered optimization problem but transformed to an usual single level optimization, thus it can be computed in reasonable time.