

Summary Table of Community Metabolic Modelling. Comparison and overview of published metabolic modelling approaches for microbial communities.

Modelling method	Modelling condition	Suitable for large community	Comments	Ref
cFBA	Steady-state, FBA	No, (pairwise analysis)	<ul style="list-style-type: none"> • Compartmentalised approach • Multi-objective function assuming fixed growth rates • Nonlinear optimisation 	[1]
SteadyCom	Steady-state, FBA	Yes	<ul style="list-style-type: none"> • Compartmentalised approach • Maximises community's specific growth rate • Less computationally demanding than cFBA 	[2]
MiCOM	Steady-state, FBA	Yes	<ul style="list-style-type: none"> • Compartmentalised approach • Maximises weighted sum of biomass fluxes of all species, then minimises sum of the squared biomass fluxes 	[3]
OptCom	Steady-state, FBA	No, (2-4 species)	<ul style="list-style-type: none"> • Bi-level and multi-objective optimisation • Maximises growth of individual species as well as the whole community 	[4]
NECom	Steady-state, FBA	No, (2-4 species)	<ul style="list-style-type: none"> • Bi-level objective optimisation • All feasible solutions are Nash equilibria of microbial community metabolic models 	[5]
Koch et al. (OptDeg)	Steady-state, FBA	No, (few species)	<ul style="list-style-type: none"> • Compartmentalised approach • Maximises the community growth rate, then optimises for optimal substrate usage (biomass yield) 	[6]
CASINO	Steady-state, FBA	Yes	<ul style="list-style-type: none"> • Maximises biomass yield of individual species, then performs iterative multi-level optimisation to maximise biomass production at the community level. 	[7]
DMMM	Temporal, FBA	Yes	<ul style="list-style-type: none"> • Extension of single species dFBA • Iteratively solves linear FBA problem for each time and species (uses Euler forward method) 	[8]
μ bialSim	Temporal, FBA	Yes	<ul style="list-style-type: none"> • To prevent negative concentrations, an augmented Euler forward method is adapted to temporarily reduce time steps 	[9]
DFBALab	Temporal, FBA	Yes	<ul style="list-style-type: none"> • Addresses infeasibility and degeneracy for exchange reaction fluxes • Needs user-defined prioritisation of shared metabolites 	[10]
ORKA	Temporal, FBA	Yes	<ul style="list-style-type: none"> • Euler forward method replaced with Runge-Kutta • Assumption of constant reaction rate relaxed over time intervals (trapezoidal rule used) 	[11]
dOptCom	Temporal, FBA	No, (2-3 species)	<ul style="list-style-type: none"> • Bi-level and multi-objective optimisation • Generally the community level objective is to maximise the community biomass concentration. 	[12]

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Brunner et al.	Temporal, FBA	Yes	<ul style="list-style-type: none"> • Uses prior solutions to inform future time steps, by simulating system forward as an ODE • Reduces the number of FBA problems that are solved 	[13]
MCM	Temporal, FBA	Yes	<ul style="list-style-type: none"> • Tool that unifies model construction, statistical evaluation, sensitivity analysis and parameter calibration • Provides versatility in terms of uptake kinetics 	[14]
COMETS	Spatiotemporal, FBA	Yes	<ul style="list-style-type: none"> • Uses biophysical models to simulate convection and diffusion of metabolites and biomass. • Biophysical models improved in recent update 	[15, 16]
BacArena	Spatiotemporal, FBA	No, (few species)	<ul style="list-style-type: none"> • Agent-based modelling approach • Can give finer resolution of communities, becomes computationally expensive for large communities 	[17]
ACBM	Spatiotemporal, FBA	No, (few species)	<ul style="list-style-type: none"> • Agent-based modelling approach • Can give finer resolution of communities, becomes computationally expensive for large communities 	[18]
Taffs et al.	Steady-state, EMA	Yes	<ul style="list-style-type: none"> • Does not require defined species and community level objective functions • Allows exploration of the entire solution space 	[19]
RedCom	Steady-state, EFVA	Yes	<ul style="list-style-type: none"> • Takes a nested (two-step) approach similar to the one by Taffs et al. but using EFVA instead of EMA • Allows for simulation of compartmentalised models 	[20]
CODY	Spatiotemporal, EMA	Yes	<ul style="list-style-type: none"> • Multiscale framework based on EMA that can be used for spatiotemporal modelling of communities. 	[21]

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