## Full SS Kernel Analysis for Toy Network

Model Toy Network with uncapped kernel of type Compact calculated on Tue 11 Jan 2022 in 1.77 seconds.

Step time limit LP tolerance Fixed value tolerance Progenitor sample size Max BFBF tree nodes BFBF random greedy sample size	60. 0.0001 0.002 20 100000 500	Stop sampling when failure rate > Minimal, Maximal LP chord counts Maximal flips to find LP chords Aspect ratios ≥ this are flattened Diameters > this not flattened Default capping radius	20 {10, 50} 25 50. 0.002
BFBF random greedy sample size	500	Default capping radius	1.
Gready search mixing fraction	0.8	Flux bounds ≥ this are taken as artificial	100.

	Constraints	Variables	Ray Yield
Stoichio, objective and range constraints	26	9	0
Remove artificial bounds, split reversibles	24	9	0
Fix 6 fluxes, revert reversibles	7	3	0
Apply mass balance and fixed objective value	0	1	0
Apply nontrivial range constraints	2	1	0
RSS after removing redundant constraints	2	1	0
RSS is closed, no capping done	2	1	0

All points in the solution space share the objective value 2.5

All 1 chords were calculated by LP for the SSK.

The maximal inscribed hypersphere diameter is 0.866025

The diameter and volume coverage ratios, between mutually similar simplices

that encloses the periphery points or the complete SSK, are  $\{100.,\ 100.\}\%$  respectively.

The mean SSK diameter is estimated to be in the range  $\{\textbf{0.866025},\,\textbf{0.866025}\}$ 

and the best value estimate is 0.866025

The sampled fraction of the SSK spanned by the

peripheral point polytope, is in the 95% confidence interval  $\{97\text{, }100\}\%$ 

2 peripheral points were found.

Assuming these to be representative, and combining with rays, extends the fixed value list to 6 items

The combined set of 0 rays span 0 of the total 0 ray dimensions.

VALIDATION TEST: Deconstruct FBA solutions (with/without artificial bounds) into the sum of a Kernel space flux, and a flux along a ray direction.

Agreement between actual and reconstituted solutions are indicated by % discrepancy of total flux, and angle in degrees between their directions in flux space.

FULL SS KERNEL		Flux vector length	% Flux mismatch	Misalignment angle deg
	Not bounded	1.2	0.	0.
	Art. bounded	1.2	0.	0.

