

# Full SS Kernel Analysis for TEST

Model TEST – iAB\_RBC\_283.mat : iAB\_RBC\_283 with uncapped kernel of type Compact  
calculated on Tue 26 Sep 2023 in 2.3 seconds.

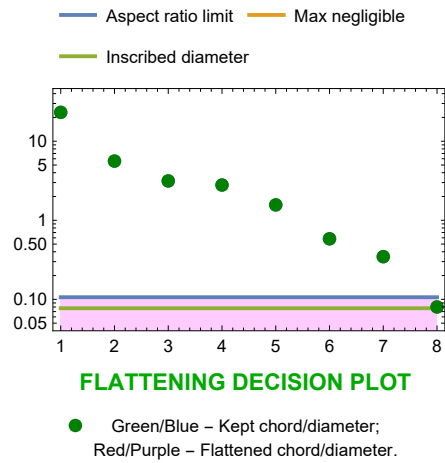
Step time limit	60.	Stop sampling when failure rate >	20
Unbuffered externals exempted	0	Minimal, Maximal LP chord counts	{10, 50}
LP tolerance	0.0001	Maximal flips to find LP chords	25
Fixed value tolerance	0.002	Aspect ratios $\geq$ this are flattened	50.
Progenitor sample size	20	Diameters > this not flattened	0.002
Max BFBF tree nodes	100000	Default capping radius	1.
BFBF random greedy sample size	500	Flux bounds $\geq$ this are taken as artificial	1000.
Greedy search mixing fraction	0.8		

	Constraints	Variables	Ray Yield
Stoichio, objective and range constraints	1281	469	0
Remove artificial bounds, split reversibles	1127	645	0
Fix 271 fluxes, revert reversibles	368	198	0
Apply mass balance and fixed objective value	0	12	0
Apply nontrivial range constraints	33	12	0
Remove prismatic rays	30	9	3
Linealities yielding ray pairs	30	8	2
RSS after removing redundant constraints	14	8	0
RSS is closed, no capping done	14	8	0

All points in the solution space share the objective value 2.93556  
All 8 chords were calculated by LP for the SSK.  
The maximal inscribed hypersphere diameter is 0.0771845  
The diameter and volume coverage ratios, between mutually similar simplices  
that encloses the periphery points or the complete SSK, are {81.1, 18.7}% respectively.  
The mean SSK diameter is estimated to be in the range {2.34032, 4.66356}  
and the best value estimate is 2.88658  
The sampled fraction of the SSK spanned by the  
peripheral point polytope, is in the 95% confidence interval {26, 31}%  
The following reactions acquired fixed directions:  
{EX\_h2o2\_e, backwards} {EX\_nh4\_e, forwards}  
62 peripheral points were found.  
Assuming these to be representative, and combining with rays, extends  
the fixed value list to 408 items  
The combined set of 4 rays span 4 of the total 4 ray dimensions.

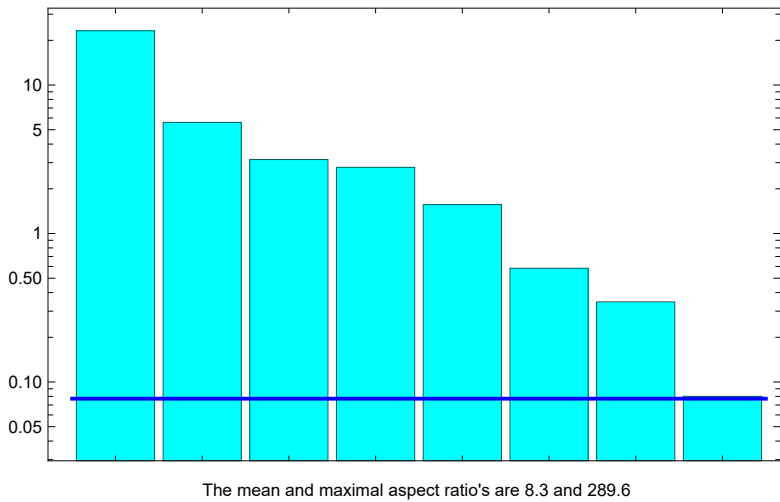
VALIDATION TEST: Deconstruct FBA solutions (with/without artificial bounds)  
into the sum of a Kernel space flux, and a flux along a ray direction.  
Agreement between actual and reconstituted solutions are indicated by % discrepancy  
of total flux, and angle in degrees between their directions in flux space.

FULL SS KERNEL		Flux vector length	% Flux mismatch	Misalignment angle deg
	Not bounded	21.5	0.	0.
	Art. bounded	1732.1	0.	0.



**MAIN ORTHOGONAL CHORD LENGTHS**

Cyan chords, magenta diameters  
Blue line is max inscribed sphere diameter



**SPLIT DIAMETERS ALONG MAIN CHORD DIRECTIONS**

Asymmetric overhang shown in light shading.

