

Parameter values

This document provides the parameter names, their biophysical meaning, their unit, and the range in which they have been sampled in the parameter space, in order to perform the Sobol's Sensitivity Analysis presented in our article: "A detailed sensitivity analysis identifies the key factors influencing enzymatic saccharification of lignocellulosic biomass".

The following parameters are used in the analysis presented in the section: Impactful parameters according to Sobol's sensitivity analysis, and the section: Effect of cellulose crystallinity

<u>Parameter</u>	<u>Biophysical meaning</u>	<u>Unit</u>	<u>Sampled range</u>
EG_rxn_rate	EG reaction rate	hour ⁻¹	1-10000
CBH_rxn_rate	CBH processive reaction rate	hour ⁻¹	1-10000
BGL_rxn_rate	BGL reaction rate	hour ⁻¹	1-10000
XYL_rxn_rate	XYL reaction rate	hour ⁻¹	0.001-1
Lignin_adhesion_rate	Number of monolignols/enzyme for non-productive adsorption	+ve integer	100-250
CBH_attachment_rate	CBH attachment rate	hour ⁻¹	0.0001-1000
Binding_affinity_cellobiose_to_EG	Inhibition binding affinity of cellobiose on EG	decimal (0-1)	0.001-1
Binding_affinity_cellobiose_to_CBH	Inhibition binding affinity of cellobiose on CBH	decimal (0-1)	0.001-1
Binding_affinity_glucose_to_EG	Inhibition binding affinity of glucose on EG	decimal (0-1)	0.001-1
Binding_affinity_glucose_to_CBH	Inhibition binding affinity of glucose on CBH	decimal (0-1)	0.001-1
Binding_affinity_glucose_to_BGL	Inhibition binding affinity of glucose on BGL	decimal (0-1)	0.001-1
Digestibility_ratio_cellulose	Digestibility ratio of crystalline to amorphous cellulose	decimal (0-1)	0.00001-0.05
Digestibility_ratio_hemicellulose	Digestibility ratio of crystalline to amorphous hemicellulose	decimal (0-1)	0.00001-0.05
Init_EG	Number of endoglucanase molecules at the start of the simulation	+ve integer	10-30
Init_CBH	Number of cellobiohydrolase molecules at the start of the simulation	+ve integer	20-80
Init_BGL	Number of β -glucosidase molecules at the start of the simulation	+ve integer	7-23
Init_XYL	Number of hemicellulase molecules at the start of the simulation	+ve integer	20-100
Pct_crystalline_cellu	Fraction of crystalline bonds in cellulose	fraction (0-1)	0-1
Pct_crystalline_hemi	Fraction of crystalline bonds in hemicellulose	fraction (0-1)	0-1

The following parameters are used in the analysis presented in the section: Role of CBH

<u>Parameter</u>	<u>Biophysical meaning</u>	<u>Unit</u>	<u>Sampled range</u>
EG_rxn_rate	EG reaction rate	hour ⁻¹	1-10000
CBH_rxn_rate	CBH processive reaction rate	hour ⁻¹	1-50
BGL_rxn_rate	BGL reaction rate	hour ⁻¹	1-10000
XYL_rxn_rate	XYL reaction rate	hour ⁻¹	0.001-1
CBH_attachement_rate	CBH attachment rate	hour ⁻¹	0.0001-1000
Binding_affinity_glucose_to_EG	Inhibition binding affinity of glucose on EG	decimal (0-1)	0.001-1
Binding_affinity_glucose_to_CBH	Inhibition binding affinity of glucose on CBH	decimal (0-1)	0.001-1
Binding_affinity_glucose_to_BGL	Inhibition binding affinity of glucose on BGL	decimal (0-1)	0.001-1
Init_EG	Number of endoglucanase molecules at the start of the simulation	+ve integer	10-30
Init_CBH	Number of cellobiohydrolase molecules at the start of the simulation	+ve integer	20-80
Init_BGL	Number of β -glucosidase molecules at the start of the simulation	+ve integer	7-23
Init_XYL	Number of hemicellulase molecules at the start of the simulation	+ve integer	20-100
Pct_crystalline_cellu	Fraction of crystalline bonds in cellulose	fraction (0-1)	0-1
Pct_crystalline_hemi	Fraction of crystalline bonds in hemicellulose	fraction (0-1)	0-1