Parameter values for "XXX"

The code version, parameter files, data files & plotting scripts used in the manuscript can be found here at XXX

The following parameters are used for the sensitivity analysis of the section XXX (crystallinity)

Parameter	Biophysical meaning	Unit	Sampled range
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_attachement_rate	CBH attachment rate	$hour^{-1}$	0.0001-1000
	Inhibition binding affinity of cellobiose on EG	decimal (0-1)	0.001-1
	Inhibition binding affinity of cellobiose on CBH	decimal (0-1)	0.001-1
	Inhibition binding affinity of glucose on EG	decimal (0-1)	0.001-1
	Inhibition binding affinity of glucose on CBH	decimal (0-1)	0.001-1
	Inhibition binding affinity of glucose on BGL	decimal (0-1)	0.001-1
$r_{c,a}$ (cellulose)	Digestibility ratio of crystalline to amorphous cellulose	decimal (0-1)	0.00001-0.05
$r_{c,a}$ (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 for the sensitivity analysis of the section XXX (CBH)

Parameter	**Biophysical meaning**	**Unit**	**Sampled range**
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
	Inhibition binding affinity of glucose on EG	decimal (0-1)	0.001-1
	Inhibition binding affinity of glucose on CBH	decimal (0-1)	0.001-1
	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