Manual

CADET Version 2.3.2

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1 CADET File Format Specifications

The CADET framework is designed to work on a file format structured into groups and datasets. This concept may be implemented by different file formats. So far readers and writers for the HDF5 and XML formats have been implemented. The choice is not limited to those two formats but can be extended as needed. The layout of such files is described in this section.

Most of the names of the groups and datasets are predefined in the C++ header file `CadetEnumeration.hpp`. Every valid CADET file needs an `input` group (see Fig. 1.2). It does not need an `output` (see Fig. 1.3) or `meta` (see Fig. 1.1) group, since those are created when results are written. If not explicitly stated otherwise, all datasets are mandatory. By convention all group names are lowercase, whereas all dataset names are uppercase. Note that the `meta` group contains input as well as output datasets.

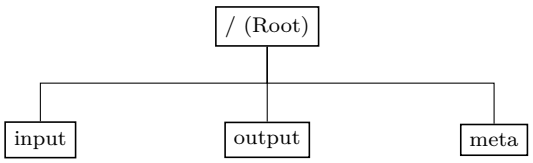

Figure 1.1: *Structure of the groups in the root group of the file format*

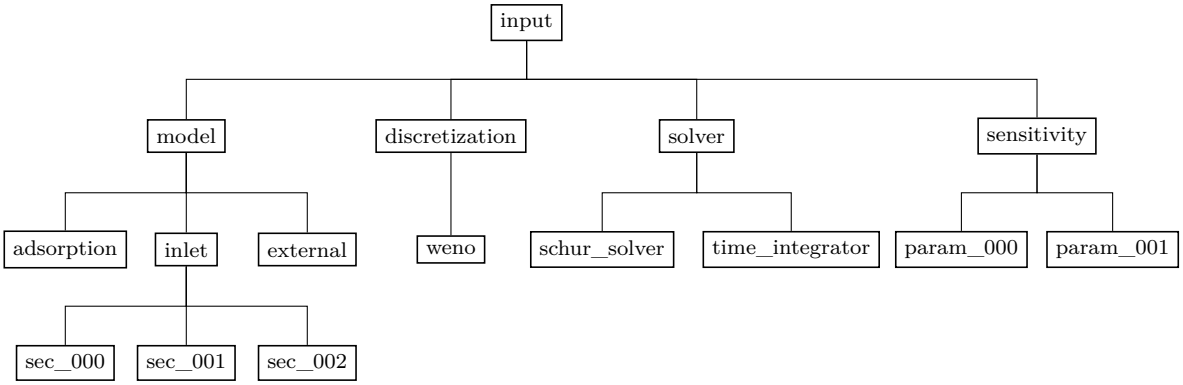

Figure 1.2: *Structure of the groups in the input part of the file format*

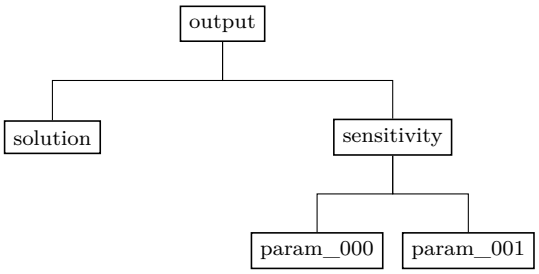

Figure 1.3: *Structure of the groups in the output part of the file format*

1.1 Description of datasets

Reference volumes are denoted by subscripts:

m^3_{Int} Interstitial volume

m^3_{MP} Bead mobile phase volume

m^3_{SP} Bead solid phase volume

1.1.1 Input group

Group /input			
Dataset	Description	Type	Range
CHROMATOGRAPHY_TYPE	Specifies the type of mass transport model	string	GENERAL_RATE_MODEL

Table 1.1: *Datasets in the* /input *group*

Group /input/model					
Dataset	Description	Unit	Type	Range	Length
NCOMP	Number of chemical components in the chromatographic media	–	int	≥ 1	1
ADSORPTION_TYPE	Specifies the type of adsorption model	–	string	See Table 1.3	1
INIT_C	A vector with initial concentrations for each comp. in the bulk mobile phase	$\mathrm{mol\,m^{-3}_{Int}}$	double	≥ 0.0	NCOMP
INIT_CP	A vector with initial concentrations for each comp. in the bead liquid phase (optional, INIT_C is used if left out)	$\mathrm{mol\,m^{-3}_{MP}}$	double	≥ 0.0	NCOMP
INIT_Q	Same as INIT_C but for the bound phase	$\mathrm{mol\,m^{-3}_{SP}}$	double	≥ 0.0	NCOMP
INIT_STATE	Full state vector for initialization (optional, INIT_C, INIT_CP, and INIT_Q will be ignored); Length NCOMP $\times$ NCOL $\times$ 2 $\times$ (NPAR + 1)	various	double	–	See description
INIT_SENS	Full state vectors of all sensitivity systems (optional, can only be used if INIT_STATE is set); Length NSENS $\times$ NCOMP $\times$ NCOL $\times$ 2 $\times$ (NPAR + 1)	various	double	–	See description
COL_DISPERSION	Axial dispersion coefficient	$\mathrm{m^2_{Int}\,s^{-1}}$	double	≥ 0.0	1 / NSEC
COL_LENGTH	Column length	m	double	> 0.0	1
COL_POROSITY	Column porosity	–	double	≥ 0.0	1
FILM_DIFFUSION	A vector with film diffusion coefficients	$\mathrm{m\,s^{-1}}$	double	≥ 0.0	NCOMP / NCOMP $\times$ NSEC
PAR_DIFFUSION	A vector with particle diffusion coefficients	$\mathrm{m^2_{MP}\,s^{-1}}$	double	≥ 0.0	NCOMP / NCOMP $\times$ NSEC
PAR_POROSITY	Particle porosity	–	double	> 0.0	1
PAR_RADIUS	Particle radius	m	double	> 0.0	1
PAR_SURFDIFFUSION	A vector with particle surface diffusion coefficients	$\mathrm{m^2_{SP}\,s^{-1}}$	double	≥ 0.0	NCOMP / NCOMP $\times$ NSEC
VELOCITY	Interstitial velocity of the mobile phase	$\mathrm{m\,s^{-1}}$	double	> 0.0	1 / NSEC

Table 1.2: *Datasets in the* /input/model *group*

Group /input/model/adsorption					
Dataset	Description	Unit	Type	Range	Length
IS_KINETIC	Selects kinetic or stationary adsorbance mode: 1 = kinetic, 0 = stationary	–	int	0/1	1
If ADSORPTION_MODEL = LINEAR:					
LIN_KA	A vector with adsorption rate constants in the linear binding model	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{m}_{\mathrm{SP}}^{-3}\,\mathrm{s}^{-1}$	double	≥ 0.0	NCOMP
LIN_KD	A vector with desorption rate constants in the linear binding model	s^{-1}	double	≥ 0.0	NCOMP
If ADSORPTION_MODEL = MULTI_COMPONENT_LANGMUIR:					
MCL_KA	A vector with adsorption rate constants in the multi component langmuir model	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$	double	≥ 0.0	NCOMP
MCL_KD	A vector with desorption rate constants in the multi component langmuir model	s^{-1}	double	≥ 0.0	NCOMP
MCL_QMAX	A vector with maximum adsorption capacities in the multi component langmuir model	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$	double	> 0.0	NCOMP
If ADSORPTION_MODEL = MOBILE_PHASE_MODULATORS:					
MPM_KA	A vector with adsorption rate constants in the mobile phase modulator model	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$	double	≥ 0.0	NCOMP
MPM_KD	A vector with desorption rate constants in the mobile phase modulator model	$\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}$	double	≥ 0.0	NCOMP
MPM_QMAX	A vector with maximum adsorption capacities in the mobile phase modulator model	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$	double	≥ 0.0	NCOMP
MPM_BETA	A vector with parameters describing the ion-exchange characteristics (IEX)	–	double	≥ 0.0	NCOMP
MPM_GAMMA	A vector with parameters describing the hydrophobicity (HIC)	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}$	double	≥ 0.0	NCOMP
If ADSORPTION_MODEL = EXTERNAL_MOBILE_PHASE_MODULATORS:					
EXTMPM_KA EXTMPM_KA_T EXTMPM_KA_TT EXTMPM_KA_TTT	All vectors with adsorption rate constants in the external function mobile phase modulator model	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$ $\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$ $\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$ $\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$	double	$-\infty - \infty$	NCOMP
EXTMPM_KD EXTMPM_KD_T EXTMPM_KD_TT EXTMPM_KD_TTT	All vectors with desorption rate constants in the external function mobile phase modulator model	$\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}$ $\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$ $\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$ $\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$	double	$-\infty - \infty$	NCOMP

Group `/input/model/adsorption` Continued

Dataset	Description	Unit	Type	Range	Length

`EXTMPM_QMAX`
`EXTMPM_QMAX_T`
`EXTMPM_QMAX_TT`
`EXTMPM_QMAX_TTT`
	All vectors with maximum adsorption capacities in the external function mobile phase modulator model	$\mathrm{mol\,m_{SP}^{-3}}$
		$\mathrm{mol\,m_{SP}^{-3}\,[T]^{-1}}$
		$\mathrm{mol\,m_{SP}^{-3}\,[T]^{-2}}$
		$\mathrm{mol\,m_{SP}^{-3}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

`EXTMPM_BETA`
`EXTMPM_BETA_T`
`EXTMPM_BETA_TT`
`EXTMPM_BETA_TTT`
	All vectors with parameters describing the ion-exchange characteristics (IEX)	–
		$\mathrm{[T]^{-1}}$
		$\mathrm{[T]^{-2}}$
		$\mathrm{[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

`EXTMPM_GAMMA`
`EXTMPM_GAMMA_T`
`EXTMPM_GAMMA_TT`
`EXTMPM_GAMMA_TTT`
	All vectors with parameters describing the hydrophobicity (HIC)	$\mathrm{m_{MP}^{3}\,mol^{-1}}$
		$\mathrm{m_{MP}^{3}\,mol^{-1}\,[T]^{-1}}$
		$\mathrm{m_{MP}^{3}\,mol^{-1}\,[T]^{-2}}$
		$\mathrm{m_{MP}^{3}\,mol^{-1}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

If `ADSORPTION_MODEL` = `EXTERNAL_LANGMUIR`:					

`EXTL_KA`
`EXTL_KA_T`
`EXTL_KA_TT`
`EXTL_KA_TTT`
	All vectors with adsorption rate constant coefficients in the External Function Langmuir model	$\mathrm{m_{MP}^{3}\,mol^{-1}\,s^{-1}}$
		$\mathrm{m_{MP}^{3}\,mol^{-1}\,s^{-1}\,[T]^{-1}}$
		$\mathrm{m_{MP}^{3}\,mol^{-1}\,s^{-1}\,[T]^{-2}}$
		$\mathrm{m_{MP}^{3}\,mol^{-1}\,s^{-1}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

`EXTL_KD`
`EXTL_KD_T`
`EXTL_KD_TT`
`EXTL_KD_TTT`
	All vectors with desorption rate constant coefficients in the External Function Langmuir model	$\mathrm{s^{-1}}$
		$\mathrm{s^{-1}\,[T]^{-1}}$
		$\mathrm{s^{-1}\,[T]^{-2}}$
		$\mathrm{s^{-1}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

`EXTL_QMAX`
`EXTL_QMAX_T`
`EXTL_QMAX_TT`
`EXTL_QMAX_TTT`
	All vectors with maximum adsorption capacity coefficients in the External Function Langmuir model	$\mathrm{mol\,m_{SP}^{-3}}$
		$\mathrm{mol\,m_{SP}^{-3}\,[T]^{-1}}$
		$\mathrm{mol\,m_{SP}^{-3}\,[T]^{-2}}$
		$\mathrm{mol\,m_{SP}^{-3}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

If `ADSORPTION_MODEL` = `STERIC_MASS_ACTION`:					
`SMA_LAMBDA`	Stationary phase capacity (monovalent salt counterions); The total number of binding sites available on the resin surface	$\mathrm{mol\,m_{SP}^{-3}}$	double	≥ 0.0	1
`SMA_KA`	A vector with adsorption rate constants in the steric mass action model	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}}$	double	≥ 0.0	`NCOMP`
`SMA_KD`	A vector with desorption rate constants in the steric mass action model	$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}}$	double	≥ 0.0	`NCOMP`

Group `/input/model/adsorption` Continued					
Dataset	Description	Unit	Type	Range	Length
`SMA_NU`	A vector with characteristic charges of the protein; The number of sites ν that the protein interacts with on the resin surface	–	double	≥ 0.0	`NCOMP`
`SMA_SIGMA`	A vector with steric factors of the protein; The number of sites σ on the surface that are shielded by the protein and prevented from exchange with the salt counterions in solution	–	double	≥ 0.0	`NCOMP`
If `ADSORPTION_MODEL` = `SELF_ASSOCIATION`:					
`SAI_LAMBDA`	Stationary phase capacity (monovalent salt counterions); The total number of binding sites available on the resin surface	$\mathrm{mol\,m_{SP}^{-3}}$	double	≥ 0.0	1
`SAI_KA1`	A vector with adsorption rate constants in the self association model	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}}$	double	≥ 0.0	`NCOMP`
`SAI_KA2`	A vector with adsorption rate constants of dimerization in the self association model	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{6}\,mol^{-(\nu_i\,+\,1)}\,s^{-1}}$	double	≥ 0.0	`NCOMP`
`SAI_KD`	A vector with desorption rate constants in the self association model	$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}}$	double	≥ 0.0	`NCOMP`
`SAI_NU`	A vector with characteristic charges ν of the protein	–	double	≥ 0.0	`NCOMP`
`SAI_SIGMA`	A vector with steric factors σ of the protein	–	double	≥ 0.0	`NCOMP`
If `ADSORPTION_MODEL` = `EXTERNAL_STERIC_MASS_ACTION`:					

`EXTSMA_KA`
`EXTSMA_KA_T`
`EXTSMA_KA_TT`
`EXTSMA_KA_TTT`
	All vectors with adsorption rate constants in the thermal steric mass action model	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}}$
		$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}\,[T]^{-1}}$
		$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}\,[T]^{-2}}$
		$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

`EXTSMA_KD`
`EXTSMA_KD_T`
`EXTSMA_KD_TT`
`EXTSMA_KD_TTT`
	All vectors with desorption rate constant coefficients in the thermal steric mass action model	$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}}$
		$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}\,[T]^{-1}}$
		$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}\,[T]^{-2}}$
		$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}\,[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

`EXTSMA_NU`
`EXTSMA_NU_T`
`EXTSMA_NU_TT`
`EXTSMA_NU_TTT`
	All vectors with characteristic charges of the protein in the thermal steric mass action model	–
		$\mathrm{[T]^{-1}}$
		$\mathrm{[T]^{-2}}$
		$\mathrm{[T]^{-3}}$
			double	$-\infty - \infty$	`NCOMP`

Group /input/model/adsorption Continued					
Dataset	Description	Unit	Type	Range	Length
EXTSMA_SIGMA EXTSMA_SIGMA_T EXTSMA_SIGMA_TT EXTSMA_SIGMA_TTT	All vectors with steric factors of the protein in the thermal steric mass action model	– $[\mathrm{T}]^{-1}$ $[\mathrm{T}]^{-2}$ $[\mathrm{T}]^{-3}$	double	$-\infty - \infty$	NCOMP
EXTSMA_LAMBDA EXTSMA_LAMBDA_T EXTSMA_LAMBDA_TT EXTSMA_LAMBDA_TTT	Stationary phase capacity (monovalent salt counterions) in the thermal steric mass action model	$\mathrm{mol\,m_{SP}^{-3}}$ $\mathrm{mol\,m_{SP}^{-3}\,[T]^{-1}}$ $\mathrm{mol\,m_{SP}^{-3}\,[T]^{-2}}$ $\mathrm{mol\,m_{SP}^{-3}\,[T]^{-3}}$	double	$-\infty - \infty$	1
If ADSORPTION_MODEL = MULTI_COMPONENT_BILANGMUIR:					
MCBL_KA1	A vector with adsorption rate constants of the first binding site type in the multi component Bi-Langmuir model	$\mathrm{m_{MP}^3\,mol^{-1}\,s^{-1}}$	double	≥ 0.0	NCOMP / 2
MCBL_KA2	A vector with adsorption rate constants of the second binding site type in the multi component Bi-Langmuir model	$\mathrm{m_{MP}^3\,mol^{-1}\,s^{-1}}$	double	≥ 0.0	NCOMP / 2
MCBL_KD1	A vector with desorption rate constants of the first binding site type in the multi component Bi-Langmuir model	$\mathrm{s^{-1}}$	double	≥ 0.0	NCOMP / 2
MCBL_KD2	A vector with desorption rate constants of the second binding site type in the multi component Bi-Langmuir model	$\mathrm{s^{-1}}$	double	≥ 0.0	NCOMP / 2
MCBL_QMAX1	A vector with with maximum adsorption capacities of the first binding site type	$\mathrm{mol\,m_{SP}^{-3}}$	double	> 0.0	NCOMP / 2
MCBL_QMAX2	A vector with with maximum adsorption capacities of the second binding site type	$\mathrm{mol\,m_{SP}^{-3}}$	double	> 0.0	NCOMP / 2

Table 1.3: *Datasets in the /input/model/adsorption group*

Group /input/model/inlet					
Dataset	Description	Unit	Type	Range	Length
NSEC	Number of sections	–	int	≥ 1	1
SECTION_TIMES	A vector with simulation times at which inlet function is discontinous; including start and end times	s	double	≥ 0.0	NSEC+1
SECTION_CONTINUITY	A vector indicating continuity of each section transition	–	int	0 (discontinuous) 1 (continuous)	NSEC-1

Table 1.4: *Datasets in the /input/model/inlet group*

Group /input/model/inlet/sec_XXX					
Dataset	Description	Unit	Type	Range	Length
CONST_COEFF	A vector with constant coefficients for inlet concentrations	$\mathrm{mol\,m_{Int}^{-3}}$	double	$-\infty - \infty$	NCOMP
LIN_COEFF	A vector with linear coefficients for inlet concentrations	$\mathrm{mol\,m_{Int}^{-3}\,s^{-1}}$	double	$-\infty - \infty$	NCOMP
QUAD_COEFF	A vector with quadratic coefficients for inlet concentrations	$\mathrm{mol\,m_{Int}^{-3}\,s^{-2}}$	double	$-\infty - \infty$	NCOMP
CUBE_COEFF	A vector with cubic coefficients for inlet concentrations	$\mathrm{mol\,m_{Int}^{-3}\,s^{-3}}$	double	$-\infty - \infty$	NCOMP

Table 1.5: *Datasets in the /input/model/inlet/sec_XXX groups*

Group /input/model/external					
Dataset	Description	Unit	Type	Range	Length
EXT_VELOCITY	Velocity of the external profile in positive column axial direction	$\mathrm{m\,s^{-1}}$	double	$-\infty - \infty$	1
EXT_PROFILE	A vector with external measurements T	[T]	double	≥ 0	Arbitrary
EXT_PROF_DELTA	A vector with distances of the external measurements (first entry must be 0.0)	m	double	≥ 0.0	Same as EXT_PROFILE

Table 1.6: *Datasets in the /input/model/external group*

Group /input/discretization					
Dataset	Description	Unit	Type	Range	Length
NCOL	Number of column (axial) discretization cells	–	int	≥ 1	1
NPAR	Number of particle (radial) discretization cells	–	int	≥ 1	1
PAR_DISC_TYPE	Specifies the discretization scheme inside the particles	–	string	EQUIDISTANT_PAR EQUIVOLUME_PAR USER_DEFINED_PAR	1
PAR_DISC_VECTOR	A vector with node coordinates for the cell boundaries	m	double	$0.0 - 1.0$	NPAR+1
RECONSTRUCTION	Type of reconstruction method for fluxes	–	string	WENO	1

Table 1.7: *Datasets in the /input/discretization group*

Group /input/discretization/weno			
Dataset	Description	Type	Range
BOUNDARY_MODEL	Boundary model type: 0 = Lower WENO order (stable), 1 = Zero weights (unstable for small D_{ax}), 2 = Zero weights for p $\neq$ 0 (stable?), 3 = Large ghost points	int	$0 - 3$
WENO_EPS	WENO ε	double	≥ 0.0
WENO_ORDER	WENO Order: 1 = standard upwind scheme, 2, 3; also called WENO K	int	$1 - 3$

Table 1.8: *Datasets in the /input/discretization/weno group*

Group /input/solver				
Dataset	Description	Unit	Type	Range
NTHREADS	Number of used OpenMP threads	–	int	≥ 1
LOG_LEVEL	Specifies the verbosity of the logging output (Only errors; warning and errors; info and warnings and errors, etc.)	–	string	ERROR WARNING INFO DEBUG1 DEBUG2 TRACE1 TRACE2
PRINT_CONFIG	Print configuration message before simulation	–	int	0/1
PRINT_PARAMLIST	Print list of parameters before simulation	–	int	0/1
PRINT_PROGRESS	Print current state of simulation	–	int	0/1
PRINT_STATISTICS	Print integrator statistics after each section	–	int	0/1
PRINT_TIMING	Print timing information after simulation	–	int	0/1
USE_ANALYTIC_JACOBIAN	Use analytically computed jacobian matrix (faster) instead of jacobian generated by algorithmic differentiation (slower)	–	int	0/1
USER_SOLUTION_TIMES	A *vector* with timepoints at which a solution is desired	s	double	≥ 0.0
WRITE_AT_USER_TIMES	Write solutions at times specified by USER_SOLUTION_TIMES (write integration timepoints otherwise)	–	int	0/1
WRITE_SOLUTION_TIMES	Write times at which a solution was produced	–	int	0/1
WRITE_SOLUTION_COLUMN_INLET	Write solutions at column inlet (boundary condition)	–	int	0/1
WRITE_SOLUTION_COLUMN_OUTLET	Write solutions at column outlet (chromatograms)	–	int	0/1
WRITE_SOLUTION_ALL	Write all (intermediate) solutions	–	int	0/1
WRITE_SOLUTION_LAST	Write full solution state vector at last time point	–	int	0/1
WRITE_SENS_COLUMN_OUTLET	Write sensitivity data at column outlet	–	int	0/1
WRITE_SENS_ALL	Write all (intermediate) sensitivity data	–	int	0/1
WRITE_SENS_LAST	Write full sensitivity state vectors at last time point	–	int	0/1

Table 1.9: *Datasets in the /input/solver group*

Group /input/solver/schur_solver			
Dataset	Description	Type	Range
GS_TYPE	Type of Gram-Schmidt orthogonalization, see IDAS guide 4.5.7.3, 41f.	int	0 (CLASSICAL_GS) 1 (MODIFIED_GS)
MAX_KRYLOV	Defines the size of the iterative linear SPGMR solver (0: MAX_KRYLOV = NCOL)	int	$0 -$ NCOL
MAX_RESTARTS	Maximum number of restarts in the GMRES algorithm. If lack of memory isn't an issue, better use a larger Krylov space than restarts	int	≥ 0
SCHUR_SAFETY	Schur safety factor; Influences the tradeof between linear iterations and nonlinear error control; see IDAS guide 2.1, 5	double	≥ 0.0

Table 1.10: *Datasets in the /input/solver/schur_solver group*

Group /input/solver/time_integrator			
Dataset	Description	Type	Range
ABSTOL	Absolute tolerance in the solution of the original system	double	> 0.0
RELTOL	Relative tolerance in the solution of the original system	double	≥ 0.0
INIT_STEP_SIZE	Factor which is multiplied by the section length to get initial integrator stepsize (0.0: IDAS default value), see IDAS guide 4.5, 36f.	double	$0.0 - 1.0$
MAX_STEPS	Maximum number of timesteps taken by IDAS (0: IDAS default = 500), see IDAS guide 4.5, 36	int	≥ 0

Table 1.11: *Datasets in the* `/input/solver/time_integrator` *group*

Group /input/sensitivity			
Dataset	Description	Type	Range
NSENS	Number of sensitivities to be computed	int	≥ 0
SENS_METHOD	Method used for computation of sensitivities; algorithmic differentiation or finite differences of order $1 - 4$	string	ad1 fd1 fd2 fd4

Table 1.12: *Datasets in the* `/input/sensitivity` *group*

Group /input/sensitivity/param_XXX			
Dataset	Description	Type	Range
SENS_NAME	Name of the parameter	string	*[1]
SENS_COMP	Component index; only for parameters defined for each component (-1 otherwise)	int	≥ -1
SENS_SECTION	Section index; only for inlet parameters (-1 otherwise)	int	≥ -1
SENS_ABSTOL	Absolute tolerance used in the computation of the sensitivities. Rule of thumb: ABSTOL / PARAM_VALUE	double	≥ 0.0
SENS_FD_DELTA	Relative disturbance Δp in finite difference sensitivity computations	double	≥ 0.0

Table 1.13: *Datasets in the* `/input/sensitivity/param_XXX` *groups*

1.1.2 Output group

Group `/output/solution`			
Dataset	Description	Unit	Type
`SOLUTION_TIMES`	Time points at which the solution is written	s	double
`SOLUTION_COLUMN`	Interstitial solution as $n_{\text{Time}} \times n_{\text{Comp}} \times n_{\text{ColCells}}$ tensor in row-major storage	$\text{mol}\,\text{m}_{\text{Int}}^{-3}$	double
`SOLUTION_PARTICLE`	Solution inside the beads as $n_{\text{Time}} \times n_{\text{ColCells}} \times n_{\text{ParCells}} \times 2 \times n_{\text{Comp}}$ tensor in row-major storage	$\text{mol}\,\text{m}_{\text{MP\&SP}}^{-3}$	double
`SOLUTION_BOUNDARY`	Flux solution as $n_{\text{Time}} \times n_{\text{Comp}} \times n_{\text{ColCells}}$ tensor in row-major storage	$\text{mol}\,\text{m}^{-2}\,\text{s}^{-1}$	double
`SOLUTION_COLUMN_OUTLET_COMP_XXX`	Component `XXX` of the solution at the column outlet	$\text{mol}\,\text{m}_{\text{Int}}^{-3}$	double
`SOLUTION_COLUMN_INLET_COMP_XXX`	Component `XXX` of the solution at the column inlet	$\text{mol}\,\text{m}_{\text{Int}}^{-3}$	double
`SOLUTION_LAST`	Full state vector of the solution at the last time point	various	double

Table 1.14: *Datasets in the `/output/solution` group*

Group `/output/sensitivity`		
Dataset	Description	Type
`SENS_COLUMN`	Interstitial solution as $n_{\text{Time}} \times n_{\text{Comp}} \times n_{\text{ColCells}} \times n_{\text{Params}}$ tensor in row-major storage	double
`SENS_PARTICLE`	Solution inside the beads as $n_{\text{Time}} \times n_{\text{ColCells}} \times n_{\text{ParCells}} \times 2 \times n_{\text{Comp}} \times n_{\text{Params}}$ tensor in row-major storage	double
`SENS_BOUNDARY`	Flux solution as $n_{\text{Time}} \times n_{\text{Comp}} \times n_{\text{ColCells}} \times n_{\text{Params}}$ tensor in row-major storage	double
`SENS_LAST`	Concatenated full state vectors of all sensitivity systems at the last time point	double

Table 1.15: *Datasets in the `/output/sensitivity` group*

Group `/output/sensitivity/param_XXX`			
Dataset	Description	Unit	Type
`SENS_COLUMN_OUTLET_COMP_YYY`	Sensitivity of component `YYY` at the column outlet with respect to parameter `XXX`	$\text{mol}\,\text{m}_{\text{Int}}^{-3}\,[\text{Param}]^{-1}$	double

Table 1.16: *Datasets in the `/output/sensitivity/param_XXX` groups*

1.1.3 Meta group

Group `/meta`			
Dataset	Description	In / out	Type
`FILE_FORMAT`	Version of the file format (defaults to 1.0 if omitted)	In	string
`CADET_VERSION`	Version of the executed CADET simulator	Out	string
`CADET_COMMIT`	Git commit SHA1 from which the CADET simulator was built	Out	string
`CADET_BRANCH`	Git branch from which the CADET simulator was built	Out	string

Table 1.17: *Datasets in the `/meta` group*

1.2 Section dependent model parameters

Some model parameters (see Table 1.18) can be assigned different values for each section. For example, the velocity the column is operated with could differ in the load, wash, and elution phases. Section dependency is recognized by specifying the appropriate number of values for the parameters (see Length in Table 1.2). If a parameter depends on the component and the section, the ordering is such that the values for the components are listed within each section (i.e., "component-major"): For example, in a three component system the ordering is `comp0sec0`, `comp1sec0`, `comp2sec0`, `comp0sec1`, `comp1sec1`, `comp2sec1`, ...

Note that single components of component dependent datasets cannot be section dependent.

Dataset	Component dependent	Section dependent
COL_DISPERSION		✓
FILM_DIFFUSION	✓	✓
PAR_DIFFUSION	✓	✓
PAR_SURFDIFFUSION	✓	✓
VELOCITY		✓

Table 1.18: *Section dependent datasets in the* `/input/model` *group*

2 Isotherms

2.1 Linear

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a c_{p,i} - k_d q_i \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

Constant	Description	Unit
k_a	Adsorption rate	$\mathrm{m}_{\mathrm{MP}}^3\,\mathrm{m}_{\mathrm{SP}}^{-3}\,\mathrm{s}^{-1}$
k_d	Desorption rate	s^{-1}

Table 2.1: *Parameters of the linear adsorption model*

2.2 Multi Component Langmuir

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a\, c_{p,i}\, q_{\max,i} \left(1 - \sum_{j=1}^{N_{\text{comp}}} \frac{q_j}{q_{\max,j}}\right) - k_d q_i \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

Constant	Description	Unit
k_a	Adsorption rate	$\mathrm{m}_{\mathrm{MP}}^3\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$
k_d	Desorption rate	s^{-1}
$q_{\max}$	Maximum adsorption capacity; Maximum concentration	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$

Table 2.2: *Parameters of the Multi Component Langmuir adsorption model*

2.3 Steric Mass Action

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a c_{p,i} \left(\Lambda - \sum_{j=1}^{N_{\text{comp}}} (\nu_j + \sigma_j)\, q_j\right)^{\nu_i} - k_d\, q_i\, c_{p,0}^{\nu_i} \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

where $c_{p,0}$ and q_0 denote the salt concentrations in the liquid and solid phase of the beads respectively. A neutrality condition compensating for the missing equation for $\frac{\mathrm{d}q_0}{\mathrm{d}t}$ is required:

$$q_0 = \Lambda - \sum_{j=1}^{N_{\text{comp}}} \nu_j q_j$$

2.4 Self Association

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = c_{p,i} \left(\Lambda - \sum_{j=1}^{N_{\text{comp}}} (\nu_j + \sigma_j)\, q_j\right)^{\nu_i} [k_{a,1} + k_{a,2} c_{p,i}] - k_d\, q_i\, c_{p,0}^{\nu_i} \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

where $c_{p,0}$ and q_0 denote the salt concentrations in the liquid and solid phase of the beads respectively. A neutrality condition compensating for the missing equation for $\frac{\mathrm{d}q_0}{\mathrm{d}t}$ is required:

$$q_0 = \Lambda - \sum_{j=1}^{N_{\text{comp}}} \nu_j q_j$$

Constant	Description	Unit
Λ	Stationary phase capacity (monovalent salt counterions); The total number of binding sites available on the resin surface	$\mathrm{mol\,m_{SP}^{-3}}$
k_a	Adsorption rate	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}}$
k_d	Desorption rate	$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}}$
ν	Characteristic charges of the protein; The number of sites ν that the protein interacts with on the resin surface	–
σ	Steric factors of the protein; The number of sites σ on the surface that are shielded by the protein and prevented from exchange with the salt counterions in solution	–

Table 2.3: *Parameters of the Steric Mass Action adsorption model*

Constant	Description	Unit
Λ	Stationary phase capacity (monovalent salt counterions); The total number of binding sites available on the resin surface	$\mathrm{mol\,m_{SP}^{-3}}$
$k_{a,1}$	Adsorption rate	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{3}\,mol^{-\nu_i}\,s^{-1}}$
$k_{a,2}$	Adsorption rate of dimerization	$\mathrm{m_{SP}^{3(\nu_i\,-\,1)}\,m_{MP}^{6}\,mol^{-(\nu_i\,+\,1)}\,s^{-1}}$
k_d	Desorption rate	$\mathrm{m_{MP}^{3\nu_i}\,mol^{-\nu_i}\,s^{-1}}$
ν	Characteristic charges of the protein; The number of sites ν that the protein interacts with on the resin surface	–
σ	Steric factors of the protein; The number of sites σ on the surface that are shielded by the protein and prevented from exchange with the salt counterions in solution	–

Table 2.4: *Parameters of the Self Association adsorption model*

2.5 Mobile Phase Modulators Langmuir

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a e^{\gamma c_{p,0}} c_{p,i}\, q_{\max,i} \left(1 - \sum_{j=1}^{N_{\text{comp}}} \frac{q_j}{q_{\max,j}}\right) - k_d\, c_{p,0}^{\beta}\, q_i \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

where $c_{p,0}$ and q_0 denote the salt concentrations in the liquid and solid phase of the beads respectively. Salt is considered to be inert, therefore

$$\frac{\mathrm{d}q_0}{\mathrm{d}t} = 0.$$

Constant	Description	Unit
k_a	Adsorption rate	$\mathrm{m_{MP}^{3}\,mol^{-1}\,s^{-1}}$
k_d	Desorption rate	$\mathrm{m_{MP}^{3\beta}\,mol^{-\beta}\,s^{-1}}$
$q_{\max}$	Maximum adsorption capacity; Maximum concentration	$\mathrm{mol\,m_{SP}^{-3}}$
γ	Hydrophobicity	$\mathrm{m_{MP}^{3}\,mol^{-1}}$
β	Describes ion-exchange characteristics	–

Table 2.5: *Parameters of the Mobile Phase Modulators Langmuir adsorption model*

2.6 External Function Multi Component Langmuir

The same as ordinary Multi Component Langmuir but with coefficients k_a, k_d, and $q_{\max}$ depending on an external quantity denoted by T:

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a(T)\, c_{p,i}\, q_{\max,i}(T) \left(1 - \sum_{j=1}^{N_{\text{comp}}} \frac{q_j}{q_{\max,j}(T)}\right) - k_d(T) q_i \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

where the dependence is modeled by a polynomial of third degree, i.e.

$$\begin{aligned} k_a(T) &= k_{a,3}T^3 + k_{a,2}T^2 + k_{a,1}T + k_{a,0}, \\ k_d(T) &= k_{d,3}T^3 + k_{d,2}T^2 + k_{d,1}T + k_{d,0}, \\ q_{\max}(T) &= q_{\max,3}T^3 + q_{\max,2}T^2 + q_{\max,1}T + q_{\max,0}. \end{aligned}$$

The quantity $T(t, z)$ is a function of time t and space z, i.e. $T\colon [0, t_{\max}] \times [0, L] \to \mathbb{R}$, which is externally given to the simulator.

Constant	Description	Unit
$k_{a,3}$	Adsorption rate	$\mathrm{m}^3_{\mathrm{MP}}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$
$k_{a,2}$		$\mathrm{m}^3_{\mathrm{MP}}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$
$k_{a,1}$		$\mathrm{m}^3_{\mathrm{MP}}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$
$k_{a,0}$		$\mathrm{m}^3_{\mathrm{MP}}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$
$k_{d,3}$	Desorption rate	$\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$
$k_{d,2}$		$\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$
$k_{d,1}$		$\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$
$k_{d,0}$		s^{-1}
$q_{\max,3}$	Maximum adsorption capacity; Maximum concentration	$\mathrm{mol}\,\mathrm{m}^{-3}_{\mathrm{SP}}\,[\mathrm{T}]^{-3}$
$q_{\max,2}$		$\mathrm{mol}\,\mathrm{m}^{-3}_{\mathrm{SP}}\,[\mathrm{T}]^{-2}$
$q_{\max,1}$		$\mathrm{mol}\,\mathrm{m}^{-3}_{\mathrm{SP}}\,[\mathrm{T}]^{-1}$
$q_{\max,0}$		$\mathrm{mol}\,\mathrm{m}^{-3}_{\mathrm{SP}}$
T	External quantity	[T]

Table 2.6: *Parameters of the External Function Multi Component Langmuir adsorption model*

2.7 External Function Steric Mass Action

The same as ordinary Steric Mass Action but with coefficients k_a, k_d, ν, σ and Λ depending on an external quantity denoted by T:

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a(T) c_{p,i} \left(\Lambda(T) - \sum_{j=1}^{N_{\text{comp}}} \left(\nu_j(T) + \sigma_j(T)\right) q_j\right)^{\nu_i(T)} - k_d(T)\, q_i\, c_{p,0}^{\nu_i(T)} \qquad \forall i = 1, \ldots, N_{\text{comp}}$$

$$q_0 = \Lambda(T) - \sum_{j=1}^{N_{\text{comp}}} \nu_j(T) q_j$$

where the dependence is modeled by a polynomial of third degree, i.e.

$$\begin{aligned} k_a(T) &= k_{a,3}T^3 + k_{a,2}T^2 + k_{a,1}T + k_{a,0}, \\ k_d(T) &= k_{d,3}T^3 + k_{d,2}T^2 + k_{d,1}T + k_{d,0}, \\ \nu(T) &= \nu_3 T^3 + \nu_2 T^2 + \nu_1 T + \nu_0, \\ \sigma(T) &= \sigma_3 T^3 + \sigma_2 T^2 + \sigma_1 T + \sigma_0, \\ \Lambda(T) &= \Lambda_3 T^3 + \Lambda_2 T^2 + \Lambda_1 T + \Lambda_0. \end{aligned}$$

The quantity $T(t,z)$ is a function of time t and space z, i.e. $T\colon [0,t_{\max}]\times[0,L]\to\mathbb{R}$, which is externally given to the simulator.

Constant	Description	Unit
$k_{a,3}$	Adsorption rate	$\mathrm{m}_{\mathrm{SP}}^{3(\nu(\mathrm{T})-1)}\,\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$
$k_{a,2}$		$\mathrm{m}_{\mathrm{SP}}^{3(\nu(\mathrm{T})-1)}\,\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$
$k_{a,1}$		$\mathrm{m}_{\mathrm{SP}}^{3(\nu(\mathrm{T})-1)}\,\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$
$k_{a,0}$		$\mathrm{m}_{\mathrm{SP}}^{3(\nu(\mathrm{T})-1)}\,\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}$
$k_{d,3}$	Desorption rate	$\mathrm{m}_{\mathrm{MP}}^{3\nu(\mathrm{T})}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$
$k_{d,2}$		$\mathrm{m}_{\mathrm{MP}}^{3\nu(\mathrm{T})}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$
$k_{d,1}$		$\mathrm{m}_{\mathrm{MP}}^{3\nu(\mathrm{T})}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$
$k_{d,0}$		$\mathrm{m}_{\mathrm{MP}}^{3\nu(\mathrm{T})}\,\mathrm{mol}^{-\nu(\mathrm{T})}\,\mathrm{s}^{-1}$
Λ_3	Stationary phase capacity (monovalent salt counterions)	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}\,[\mathrm{T}]^{-3}$
Λ_2		$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}\,[\mathrm{T}]^{-2}$
Λ_1		$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}\,[\mathrm{T}]^{-1}$
Λ_0		$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$
ν_3	Characteristic charges of the protein	$[\mathrm{T}]^{-3}$
ν_2		$[\mathrm{T}]^{-2}$
ν_1		$[\mathrm{T}]^{-1}$
ν_0		–
σ	Steric factors of the protein	$[\mathrm{T}]^{-3}$
σ		$[\mathrm{T}]^{-2}$
σ		$[\mathrm{T}]^{-1}$
σ		–
T	External quantity	[T]

Table 2.7: *Parameters of the External Function Steric Mass Action adsorption model*

2.8 External Function Mobile Phase Modulators Langmuir

The same as ordinary Mobile Phase Modulators Langmuir but with coefficients $k_a, k_d, q_{\max}, \gamma$ and β depending on an external quantity denoted by T:

$$\frac{\mathrm{d}q_i}{\mathrm{d}t} = k_a(T)e^{\gamma(T)c_{p,0}}c_{p,i}\,q_{\max,i}(T)\left(1-\sum_{j=1}^{N_{\mathrm{comp}}}\frac{q_j}{q_{\max,j}(T)}\right) - k_d(T)\,c_{p,0}^{\beta(T)}\,q_i \qquad \forall i=1,\ldots,N_{\mathrm{comp}}$$

where the dependence is modeled by a polynomial of third degree, i.e.

$$\begin{aligned}
k_a(T) &= k_{a,3}T^3 + k_{a,2}T^2 + k_{a,1}T + k_{a,0},\\
k_d(T) &= k_{d,3}T^3 + k_{d,2}T^2 + k_{d,1}T + k_{d,0},\\
q_{\max}(T) &= q_{\max,3}T^3 + q_{\max,2}T^2 + q_{\max,1}T + q_{\max,0},\\
\gamma(T) &= \gamma_3T^3 + \gamma_2T^2 + \gamma_1T + \gamma_0,\\
\beta(T) &= \beta_3T^3 + \beta_2T^2 + \beta_1T + \beta_0.
\end{aligned}$$

The quantity $T(t,z)$ is a function of time t and space z, i.e. $T\colon [0,t_{\max}]\times[0,L]\to\mathbb{R}$, which is externally given to the simulator.

2.9 Multi Component Bi-Langmuir

The Multi Component Bi-Langmuir model adds a second type of binding site q_i^B to the Langmuir model without allowing an exchange between the two sites q_i^A and q_i^B. Therefore, there are no competitivity effects

Constant	Description	Unit
$k_{a,3}$	Adsorption rate	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$
$k_{a,2}$		$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$
$k_{a,1}$		$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$
$k_{a,0}$		$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$
$k_{d,3}$	Desorption rate	$\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-3}$
$k_{d,2}$		$\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-2}$
$k_{d,1}$		$\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}\,[\mathrm{T}]^{-1}$
$k_{d,0}$		$\mathrm{m}_{\mathrm{MP}}^{3\beta}\,\mathrm{mol}^{-\beta}\,\mathrm{s}^{-1}$
$q_{\max,3}$	Maximum adsorption capacity; Maximum concentration	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$
$q_{\max,2}$		$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}\,[\mathrm{T}]^{-2}$
$q_{\max,1}$		$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}\,[\mathrm{T}]^{-1}$
$q_{\max,0}$		$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$
γ_3	Hydrophobicity	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,[\mathrm{T}]^{-3}$
γ_2		$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,[\mathrm{T}]^{-2}$
γ_1		$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,[\mathrm{T}]^{-1}$
γ_0		$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}$
β_3	Describes ion-exchange characteristics	$[\mathrm{T}]^{-3}$
β_2		$[\mathrm{T}]^{-2}$
β_1		$[\mathrm{T}]^{-1}$
β_0		–
T	External quantity	[T]

Table 2.8: *Parameters of the External Function Mobile Phase Modulators Langmuir adsorption model*

between the two types of binding sites and they have independent capacities.

$$\frac{\mathrm{d}q_i^A}{\mathrm{d}t} = k_a^A\, c_{p,i}\, q_{\max,i}^A \left(1 - \sum_{j=1}^{N_{\mathrm{comp}}} \frac{q_j^A}{q_{\max,j}^A}\right) - k_d^A\, q_i^A \qquad \forall i = 1, \ldots, N_{\mathrm{comp}}$$

$$\frac{\mathrm{d}q_i^B}{\mathrm{d}t} = k_a^B\, c_{p,i}\, q_{\max,i}^B \left(1 - \sum_{j=1}^{N_{\mathrm{comp}}} \frac{q_j^B}{q_{\max,j}^B}\right) - k_d^B\, q_i^B \qquad \forall i = 1, \ldots, N_{\mathrm{comp}}$$

Constant	Description	Unit
k_a^A	Adsorption rate of first binding site type	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$
k_a^B	Adsorption rate of second binding site type	$\mathrm{m}_{\mathrm{MP}}^{3}\,\mathrm{mol}^{-1}\,\mathrm{s}^{-1}$
k_d^A	Desorption rate of first binding site type	s^{-1}
k_d^B	Desorption rate of second binding site type	s^{-1}
$q_{\max}^A$	Maximum adsorption capacity; Maximum concentration of first binding site type	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$
$q_{\max}^B$	Maximum adsorption capacity; Maximum concentration of second binding site type	$\mathrm{mol}\,\mathrm{m}_{\mathrm{SP}}^{-3}$

Table 2.9: *Parameters of the Multi Component Bi-Langmuir adsorption model*