

### 3 INPUT PREPARATION

#### 3.1 General

The application of MOUSER requires specification of numerous input parameters. The organization of the primary input file is summarized in Table 3.1. The values for various integer flags are summarized in Table 3.2, with brief descriptions of the line-by-line input following. A more detailed discussion of procedures for specifying key parameters is provided in Chapter 4 in the context of specific applications.

**Table 3.1 Summary of MOUSER input parameters**

Line	Type	Meaning	Comment
1	CHAR	Comment (up to 40 characters)	
2-4	INT	Integer flags for problem classification	
5	CHAR	Name of summary output file	
6	CHAR	Name of data output file(s)	
7-8	INT	Integer flags for domain configuration	
9	REAL	Output parameters (space and time)	
10	REAL	Media physical properties	
11	REAL	Advection parameters	
12	REAL	Dispersivity and tortuosity	Solute-independent
Transport parameters for each solute (S)			
S1	CHAR	Solute name	
S2	REAL	Entrance BC parameter(s)	number depends on BC
S3	REAL	Exit BC parameter(s)	number depends on BC
S4	REAL	Initial condition	
S5	REAL	Diffusion coefficient	
S6	REAL	Aqueous decay constant	
S7	REAL	Sorbed phase decay constant	
S8	REAL	Sorption capacity	linear equilibrium sorption
Reaction parameters (number of lines depends on reaction system)			
	REAL	Nonlinear isotherm parameters (1-3)	Kinetic or equilibrium
	REAL	Sorption rate constant	Kinetic sorption only
	REAL	Decay product conversation ratio	Sequential decay only
	REAL	Cation exchange parameters	Multiple lines of input
Calibration parameters			
	INT	Number of observations	
	REAL, INT	Dependent variable and number of dependent variable observations	One line for each observation
	INT	Solute number(s) corresponding to observations	One line for each observation

CHAR - character (40 max), INT = Integer, REAL = real (double precision)

### 3.2 Units

For problems that do not involve nonlinear reactions, the user may specify parameters using any consistent set of units. For some nonlinear reactions, changes in the mass concentration units used for initial/boundary conditions may require redefinition of reaction constants. For simplicity, the following units convention is recommended for all variables except density and sorption capacity:

- Time [T]: *days* (d)
- Distance [L]: *meters* (m)
- Aqueous mass concentration [ $\text{ML}^{-3}$ ]: *milligrams per liter* (mg/L)

The bulk density [ $\text{ML}^{-3}$ ] and linear sorption equilibrium constant [ $\text{M}^{-1}\text{L}^3$ ] are commonly reported in units of g/mL and mL/g, respectively. (For models based on linear equilibrium sorption, any consistent units can be used as long as the product is dimensionless.)

In the program output, the aqueous concentration is expressed in the same units as the output (mg/L recommended). The instantaneous flux [ $\text{ML}^{-2}\text{T}^{-1}$ ] output is expressed in units equivalent to the input flow velocity multiplied by the aqueous concentration. The units of the output total concentration [ $\text{MM}^{-1}$ ] are equivalent to the aqueous concentration divided by the bulk density (e.g., mg/kg when concentration is in mg/L and bulk density is in g/ml).

### 3.3 Line-by-line parameter descriptions: General

#### Lines 1: Remark

*Line 1* contains a text string that is written to the top of the summary output file.

#### Line 2: General problem description

*Line 2* contains integer flags that provide information about the structure of the program. A detailed summary is provided in Table 3.2, with a general description provided below:

- *isorp*. This input determines the form of the sorption model(s). Specification of *isorp* > 0 requires additional reaction input
- *isthrm*. This input determines the form of the sorption equilibrium isotherm. Specification of *isthrm* > 0 requires additional reaction input.
- *idecay*. This input identifies the appropriate decay model: single solute (*idecay* = 0) or multi-solute with reaction products (*idecay* = 1). Specification of *idecay* > 0 requires additional reaction input

#### Line 3: Output control

*Line 3* contains integer flags that determine the form of the program output. MOUSER computes the contaminant aqueous concentration, instantaneous flux, cumulative mass per area, and total (sorbed plus aqueous) concentration for a set of spatial locations and times specified by the user. Output is configured based on the values of *iprof* and *iout*, as summarized in Table 3.3. Setting a nonzero value of the variable *icalib* generates

additional output processing to support calibration using an external program (this feature is under development; *icalib* is currently ignored by MOUSER).

**Table 3.2 Integer flags on line 2**

Line	Variable	Values	Meaning
2	<i>isorp</i> : sorption scenario	0	equilibrium
		1	first-order nonequilibrium
		2	reserved for future use
		3	multi-solute cation exchange
2	<i>isthrm</i> : sorption isotherm	0	linear (Eq. 2.17)
		1	Freundlich (Eq. 2.18)
		2	Langmuir (Eq. 2.19)
		3	Toth (Eq. 2.20)
2	<i>idecay</i> : decay scenario	0	single-solute decay
		1	multi-solute parent/daughter decay

**Table 3.3 Integer flags on line 3**

Line	Variable	Value	Meaning
3	<i>iprof</i> : output type	0	temporal (single location, multiple times)
		1	spatial (single time, multiple locations)
		2	temporal + spatial at end of simulation
		3	spatial, steady-state (under development)
3	<i>iout</i> : output variables	0	time/space, aqueous concentration
		1	time, flux
		2	time, cumulative mass
		3	time, aq. concentration, flux, cum. mass
		4	space, total concentration
		5	space, aq. concentration, total concentration
3	<i>icalib</i> : calibration variable	0	simulation without calibration
		1	simulation with calibration

#### Line 4: Numerical methods

Line 4 contains integer flags that control the numerical solution technique.

- *method*. The *method* flag indicates whether the transport solution procedure is based on analytical, finite layer (numerical inversion of Laplace-transformed solution) or finite difference/element techniques, as summarized in Table 3.4.
- *iflow*. The *iflow* flag indicates how velocities are calculated, as summarized in Table 3.4.

- *itrans*. The *itrans* flag indicates which solution technique is used when a numerical solution to the advective-dispersive equation is specified (*method* = 2), as summarized in Table 3.4. The input is ignored if the analytical (*method* = 0) or inverse Laplace (*method* = 1) algorithms are specified.
- *ireact*. The *ireact* flag indicates which solution technique is used to solve the reaction equations when operating splitting is used (*method* = 3).

**Table 3.4 Integer flags on line 4**

Line	Variable	Values	Meaning
4	<i>method</i> : calculation method	0	analytical
		1	inverse Laplace
		2	numerical
4	<i>iflow</i> : velocity calculation	0	<i>v</i> calculated using Eq. 2.2a
		1	<i>v</i> calculated using Eq. 2.2b
		2	<i>v</i> calculated using Eq. 2.2c
		3	<i>v</i> input directly
4	<i>itrans</i> : transport algorithm	0	implicit finite element, split-op
		1	explicit finite difference, coupled
		2	total variation diminishing, split-op
4	<i>ireact</i> : reaction algorithm	0-3	depends on reaction system

**Line 5: General output file**

*Line 5* contains names of the file to which general program output is written, including a summary of the input parameters, various intermediate calculated variables, and (for numerical models) a summary of mass balance calculations.

**Line 6: Numerical output file(s)**

*Line 6* contains the name of the file(s) to which the data output (numbers only) is written. A single file is used when the specified output profile is either temporal only (*iprof* = 0) or spatial only (*iprof* = 1 or 2). When both temporal and spatial profiles are requested (*iprof* = 3), two file names must be provided, with the first corresponding to the temporal output and the second used for spatial output at the end of the simulation.

**Line 7: Discretization parameters**

*Line 7* gives the number of transport solutes and information regarding space and time discretization.

- *nsolut*. The value of *nsolut* determines the individual solutes for which transport is modeled. For each solute a separate block of input must be provided beginning on line 13. Also, the number of solutes must be compatible with the specified reaction type (combination of *isorp* and *idecay*).

- *nx*. The meaning of *nx* depends on the solution technique. For the analytical or finite layer methods (*method* = 0 or 1), *nx* determines the number of spatial locations for which output is generated when a spatial profile is specified (*iprof* = 1). For a temporal profile (*iprof* = 0), the program sets *nx* = 1 regardless of the user-supplied input. Because the analytical and finite layer solutions are unaffected by the spatial discretization, *nx* impacts only the quality of spatial plots generated from the results. Typically, 50-100 output points will be adequate to generate a smooth plot. For finite difference or finite solutions (*method* = 2), spatial discretization is required for the solution procedure and the grid size impacts the accuracy of the solution (see discussion in Chapter 4). For the finite element solution (*itrans* = 0), if the specified number of nodes is even, the program will add an additional node.
- *nt*. The value of *nt* determines the minimum number of time steps. For the analytical or inverse Laplace solutions, the number of time steps corresponds to the number of desired temporal output points. Typically, 50-100 output points will be adequate to generate a smooth plot. Because the accuracy of the numerical solution is sensitive to spatial and temporal discretization (see Chapter 4), the required number of time steps may be greater than the number of desired output points. For this case, the parameter *nti* (below) is used to control the number of output points.
- *nti*. The value of *nti* determines the time step increment used to generate output. For the analytical and inverse Laplace solutions, *nti* will normally be set 1, which implies that calculations are performed only at times for which output is desired. For numerical solutions, less output may be desired. Increasing *nti* will correspondingly reduce the number of output points (e.g., *nti* = 3 means that output will be generated at every third time step).

### Line 8: Boundary condition flags

Line 8 contains integer flags that determine the form of the boundary conditions:

- *ienter*. Seven possible entrance BCs are available, as summarized in Table 3.5. Additional input must be provided in the solute-specific blocks.
- *iexit*. Four exit BC options are available in the current version, as summarized in Table 3.5. Additional input must be provided in the solute-specific blocks.

A discussion of BC selection for specific applications is provided in Chapter 4.

### Line 9: Output points

The spatial and temporal coordinates for the program output must be provided:

- *Initial output time* [T]. For most problems involving temporal profiles, the appropriate value is zero, although the user may specify a later time if viewing of the entire simulation period is not desired. For spatial profiles, the initial time should equal the final output time.
- *Final output time* [T]. The value entered for this variable determines the length of the simulation period.
- *Initial output distance* [L]. For most problems involving spatial profiles, the appropriate value is zero, although the user may specify a nonzero distance if viewing of a subset of the domain is desired. For temporal profiles, the initial distance should equal the final output distance.

- *Final output distance* [L]. For most problems involving spatial profiles, the appropriate value is the domain length, although the user may specify a shorter distance if viewing of the entire domain is not desired. For temporal profiles, the final distance should equal the initial distance, with the most likely selection being the domain length.

**Table 3.3 Boundary condition flags**

Line	Variable	Values	Meaning
8	<i>ienter</i> : entrance BC	0	constant concentration (Eq. 2.6)
		1	Danckwerts (Eq. 2.7)
		2	exponential trend (Eq. 2.9)
		3	linear trend (Eq. 2.10)
		4	quadratic trend (Eq. 2.10)
		5	finite mass (no decay) (Eq. 2.8a)
		6	finite mass with decay (modified Eq. 2.8)
8	<i>ixit</i> : exit BC	0	zero gradient (finite) (Eq. 2.13)
		1	zero gradient (semi-infinite) (Eq. 2.12)
		2	constant concentration (Eq. 2.11)
		3	mixing zone (Eq. 2.14)

**Line 10: Domain physical parameters**

The user is required to provide various physical properties of the domain:

- *Domain length* ( $L$ ) [L]. For most scenarios, the user will request output for the end of the model domain, and the values entered in lines 9 and 10 will be identical. It is possible, however, that the user may request output for a location interior to the domain. Regardless of the output locations, correct specification of the domain length is important because it determines the location and relative influence of the exit BC. When a semi-infinite domain is desired (to reduce boundary effects) in a numerical simulation, it is common to increase the domain length by a factor of 3-5 beyond the point where output is desired.
- *Porosity* ( $n$ ) [dimensionless]. The specified porosity must be between 0.0 and 1.0 or an error message will be generated. Suggested ranges for other types of porous media are given in standard groundwater texts (e.g., Domenico and Schwartz, 1998). A solid material (e.g., sheet pile) may also be simulated by specifying a porosity of 1.0.
- *Bulk density* ( $\rho_b$ ) [ $\text{ML}^{-3}$ ]. This parameter defines the density of the porous media when dry (including void space). It is currently used by MOUSER only as part of expressions related to the sorption process. The solid density ( $\rho_s$ , excludes voids) for most porous media is readily measured; a reasonable default value for earthen materials is 2.65 g/mL. The bulk density can be computed from a known solid density as  $\rho_b = (1 - n)\rho_s$ .

**Line 11: Advection parameters**

The advective velocity ( $v$ ) can be determined by several approaches, depending on the value of *iflow* specified in Line 4. Depending on this value, the user is required to provide the following information according to one of the following schemes:

- *Hydraulic conductivity* ( $K$ ) [ $\text{LT}^{-1}$ ] and *hydraulic gradient* ( $i$ ) (*iflow* = 0). The velocity is then computed by the programs as  $v = Ki/n$ . This approach may be the most intuitive for barrier applications. The hydraulic gradient may be interpreted as the difference in the piezometric head across the domain, divided by the barrier length. A positive gradient implies that a higher value on the entrance side of the barrier, while a negative value corresponds to a higher value on the exit side. Negative gradients may be specified, for example, if a pumping well is located on the inside of a contained area. Estimates of the hydraulic gradient are usually obtained from field measurements, although a useful application of the model may be to perform sensitivity analysis to assess the impact of pumping within a containment system. Under natural gradient conditions, typical values of the gradient may range from 0.001 to 0.05 (dimensionless), while higher values would be expected when pumping wells are operating.
- *Volumetric flow rate* ( $Q$ ) [ $\text{L}^3\text{T}^{-1}$ ] and *cross-sectional area* ( $A$ ) (*iflow* = 1). The velocity is then computed by the program as  $v = Q/nA$ . This approach may be the most intuitive for application to soil column experiments.
- *Specific discharge* ( $q$ ) [ $\text{LT}^{-1}$ ] (also termed Darcy velocity or flow per area) (*iflow* = 2). The velocity is then computed by the programs as  $v = q/n$ .
- *Velocity* ( $v$ ) [ $\text{LT}^{-1}$ ] (*iflow* = 3). This is the most straightforward approach, used when the actual fluid velocity is known.

**Line 12: Physical dispersion/diffusion parameters**

The value of the dispersion coefficient is computed by the program according to Eq. 2.3. Two of the three necessary parameters are properties of the domain, not the solute:

- *Dispersivity* ( $\alpha_l$ ) [L]. The dispersivity is a property of the porous medium that determines the degree of hydrodynamic mixing that contributes to dispersive transport, as expressed in Eq. 2.3. In general, the appropriate dispersivity is scale dependent; i.e., as the domain length is increased, the dispersivity should be increased. A reasonable starting point for estimating dispersivity is 5-10% of the domain length. A more detailed discussion of dispersion is provided in Chapter 4.
- *Diffusion hindrance* ( $H_p$ ) [dimensionless]. The hindrance parameter is used to modify the solute-specific diffusion coefficient to account for the porous media structure, as expressed in Eq. 2.3. Predictions for advection-dominated problems will normally be insensitive to the hindrance. Diffusion-dominated simulations are very sensitive to the specified hindrance; however, estimation of  $H_p$  is difficult. A typical value for the hindrance of earthen materials is 1.5, while a conservative (more rapid) prediction of diffusion-dominated transport may be generated by setting the hindrance to 1.0. A solid barrier may be represented by setting the hindrance parameter to 1.0 and reinterpreting the diffusion coefficient (line S5 below) as the effective diffusion coefficient for the solid material. Further discussion is provided in Chapter 4.

### 3.4 Line-by-line parameter descriptions: solute blocks

Beginning with Line 13, a block of input data must be provided for each of the *nsolut* solutes specified in Line 7. In the summary given below, the prefix *S* is used to denote the solute-specific section of the input file.

#### Line S1: Solute name

A character variable of up to 40 characters in length must be provided at the beginning of each solute block.

#### Line S2: Entrance boundary condition

Depending on the entrance BC specified, up to 4 parameters may be need. Only the required parameter must be supplied by the user, in the order given below:

- *Initial contaminant source concentration ( $C_0$ )* [ $\text{ML}^{-3}$ ]. This parameter is required for all entrance BC scenarios.
- *Entrance BC decay rate ( $\lambda_s$ )* [ $\text{T}^{-1}$ ]. This parameter is required for an exponentially decaying source (entrance BC option 2) or a finite mass BC with decay (*ienter* = 6).
- *Entrance BC slope ( $P_1$ )* [ $\text{ML}^{-3}\text{T}^{-1}$ ]. This parameter is used for the linear or quadratic BC functions (*ienter* = 3 or 4).
- *Entrance BC quadratic term ( $P_2$ )* [ $\text{ML}^{-3}\text{T}^{-2}$ ]. This parameter is used for the quadratic BC function (*ienter* = 4).
- *Entrance finite mass zone thickness ( $H_f$ )* [L]. This parameter is used for the entrance finite mass conditions (*ienter* = 5 or 6).

#### Line S3: Exit boundary condition

For all options except the “mixing zone” case, the program reads the value of a specified boundary concentration or gradient. (Since the current program supports nonzero values only for *iexit* = 0 with zero advection, the program may “override” the input and assign a value of zero for this variable). For the “mixing zone” approach (*iexit* = 3), a different set of variables must be supplied.

- *Boundary concentration/gradient* [ $\text{ML}^{-3}$  or  $\text{ML}^{-4}$ ]. The current program supports nonzero input only for *iexit* = 2 and zero hydraulic gradient (line 12). For other scenarios, (except *iexit* = 3), a single dummy variable (any value) must be supplied, which is ignored by the program. For the mixing zone scenario (*iexit* = 3), different input is required, as defined below.
- *Barrier area ( $A$ )* [ $\text{L}^2$ ]. This parameter defines the cross-section area of the barrier (yz plane) for use with the exit mixing zone BC.
- *Exit mixing zone volume ( $V_e$ )* [ $\text{L}^3$ ]. This parameter defines the volume of the pore fluid contained in the exit mixing zone.
- *Exit mixing zone flow rate ( $Q_e$ )* [ $\text{L}^3\text{T}^{-1}$ ]. This parameter defines the rate at which fluid is removed from the exit mixing zone.

#### Line S4: Initial condition

A single value for the solute initial condition ( $C_i$ ) [ $\text{ML}^{-3}$ ] must be supplied. For many problems of interest, the appropriate value is zero. Several of the analytical solution algorithms do not support nonzero initial conditions; for these scenarios, the input is ignored, a zero value is assigned, and a warning message is generated.



**Line S5: Contaminant diffusion and decay properties**

Several chemical properties of must be provided for each solute:

- *Liquid diffusion coefficient ( $D_d$ ) [ $L^2T^{-1}$ ]*. The diffusion coefficient refers to molecular diffusion of the solute in a dilute aqueous solution and is typically on the order of  $8.64 \times 10^{-5} \text{ m}^2/\text{d}$  ( $10^{-5} \text{ cm}^2/\text{s}$ ) for most organic solutes. Methods for estimating liquid diffusion coefficients are discussed in Lyman et al. (1990) and Cussler (1996). The liquid diffusion coefficient is divided by the hindrance to yield an “effective” diffusion constant, as expressed in Eq. 2.3. Further discussion is provided in Chapter 4.
- *Aqueous decay rate ( $\mu_a$ ) [ $T^{-1}$ ]*. Decay may occur in both the aqueous and sorbed phases, although sorbed phase decay is usually considered only for radionuclides. For many scenarios of interest, solute decay is negligible and a zero value is appropriate. There are many exceptions, however, including radionuclide transport, engineered reactions in permeable reactive barriers, and biotransformation scenarios. In particular, for low permeability barriers, even small decay rates may significantly impact the solutions due to the long residence times inside barriers. The range of potential values for decay constants is large. Useful reviews are presented by Moody (1982) for radionuclides, Vogel et al. (1987) for abiotic reactions, and Tratnyek et al. (1997) for iron-based treatment walls.
- *Sorbed phase decay rate ( $\mu_s$ ) [ $T^{-1}$ ]*. As indicated above, the use of a nonzero decay rate for the sorbed phase is relatively uncommon and generally limited to radionuclides.
- *Distribution coefficient ( $K_d$ ) [ $L^3M^{-1}$ ]*. The distribution coefficient is the only parameter needed to define the linear isotherm ( $isthrm = 0$ ). It is usually obtained from batch or column experiments with the medium and contaminants of concern. For some organic solutes, literature correlations may be used to estimate the sorption capacity based on the contaminant properties and organic content of the media (e.g., see Fetter, 1993). The variable is read but ignored if a nonlinear isotherm is specified.

**3.5 Line-by-line parameter descriptions: Reaction parameters**

For many problems of interest, no further input is required. However, for some of the MOUSER reaction scenarios, additional information must be included at the end of the input file. The specific parameters depend on the nature of the sorption process (determined by *isorp* and *isthrm* in Line 2) and decay reaction(s) (determined by *idecay* in Line 2).

**Nonlinear sorption parameters**

Depending on the sorption options specified by *isthrm* (Line 2), up to three isotherm parameters must be provided. These parameters are typically estimated from laboratory batch tests.

- *Freundlich parameters*. If the nonlinear Freundlich isotherm is specified ( $isthrm = 1$ ), values for the capacity  $K_f$  [ $L^3M^{-1}$ ] $^{1/n_f}$  and exponent ( $n_f$ ) parameters must be supplied (Eq. 2.18). One line of input used for each parameter, with multiple solutes placed on the same line (in numerical order).

- *Langmuir parameters.* If the nonlinear Langmuir isotherm is specified (*isthrm* = 2), the two isotherm parameters must be supplied:  $Q_0$  [MM<sup>-1</sup>, units of sorbed phase concentration] and  $b$  [L<sup>3</sup>M<sup>-1</sup>, inverse of concentration units] from (Eq. 2.19). One line of input used for each parameter, with multiple solutes placed on the same line (in numerical order)
- *Toth parameters.* If the nonlinear Toth isotherm is specified (*isthrm* = 3), three isotherm parameters must be supplied:  $Q_0$ ,  $b$ , and  $n_T$  [dimensionless] (Eq. 2.20). One line of input used for each parameter, with multiple solutes placed on the same line (in order of solute numbering).

### Reaction product conversion ratios

If the multi-solute decay model is specified (*idecay* = 1), the production of decay products is determined by the product of the parent compound decay rate ( $\mu$  in Line S5) and a product conversion factor ( $\beta_i$ ) [dimensionless], which accounts for multiple product pathways and/or differences in molecular weight. The (*nsolut* - 1) conversion parameters are placed in one line of input (in order of solute numbering).

### Sorption rate constant

When a first-order mass transfer model is specified (*isorp* = 1 on Line 2), the *sorption rate constant* ( $\alpha$ ) [T<sup>-1</sup>] must be supplied. One line of input is required, with the parameters for multiple solutes placed in numerical order. In general, it is difficult to obtain *a priori* estimates of sorption rate constants; laboratory experimentation is normally required.

### Cation exchange parameters

For the competitive cation exchange model, a number of additional parameters must be supplied, as discussed in Section 2.6 and Chapter 4:

- The first line of additional input contains the *molecular weight* (g/mole), *cation charge*, and *initial sorbed phase concentration* [mg/kg] for the reference solute, which is typically sodium (Na).
- For each of the remaining (*nsolut* - 1) solutes, one line of input must be supplied that contains the *molecular weight* (g/mole), *cation charge*, *initial sorbed phase concentration* [mg/g], and *selectivity coefficient* [dimensionless, with respect to the reference solute].
- After the solute-specific parameters, a single line of input is supplied that contains the aqueous phase *anion activity* [meq/L], which is assumed constant within the domain and influent fluid.

## 3.5 Line-by-line parameter descriptions: Calibration parameters

MOUSER is designed to support model calibration using third-party software such as PEST, UCODE, or OSTRICH. None of the calibration tasks are performed by MOUSER, but output must be configured to match the available observation data. The calibration information is the last component of the input file, appearing after the reaction parameters. The first lines of input contains the number of observations used for calibration (*nobs*). Following the initial line, two blocks of input are required, with one line for each observation:

- The first block of input contains the value of the dependent variable (space or time) and the number of solutes for which a data point is provided. For multi-solute scenarios, this structure allows for the case where observations include only a subset of the modeled solutes.
- After the first block of *nobs* lines of input, a second block of *nobs* lines is provided that contains the number(s) of each solute for which observation data are provided. The number of entries in each line should correspond to the number of solutes given in the corresponding line of previous block of input.

The input provided in the calibration section is used by MOUSER to adjust the program output from a uniformly spaced distance/time grid to a set of discrete output puts that match the data. The form of the output will conform to the specifications given by the *iprof* and *iout* variables described above. The actual observation data are not used by MOUSER; file and data formatting requirements for the observations are determined by the calibration software.