Table 1a
Input File Variable Explanation - Forward Execution

Explanation
Input file is ASCII text.
Input file content is in the two columns below heading "Model input", in black font.
Comments, units, and variable explanations are in blue font.
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Variable names in the first column are case-sensitive, numeric values in the second column are in free format. The space or tab separated pairs (name, value)
All output instructions must be within block OUTPUT... ENDOUTPUT at the end of the file.
Units are shown as mass (M), length (L), time (T), energy (J), power (W), temperature (K)

Model input		*Units*	*Default Value Units*	*Allowed Value*	*Explanation*
NOTE					
	this is an example input file			any text, numbers	Descriptive note
ENDNOTE					
Mode	forward	-		inverse, forward	Forward or inverse execution. Any other word than "inverse" results in forward execution. If "inverse", all input outside the block INVERSE is ignored. If this line is omitted, execution is forward to assure backward compatibility with T3D8.
Model	2			1,2,3,4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3	use Model 1, 2, 3, 4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3
transport	heat*			mass, heat	Simulate mass or heat transport, default is mass (any other word than "heat" means mass transport simulation, i.e. " heat* " results in mass transport simulation).
TOL	1.00E-10	-			tolerance limit for Laplace transform
Ktol	1.00E-03	-			tolerance limit for z-summation
Ntol	1.00E-03	-			tolerance limit for y-summation
Nmin	15	-			min number of y-summation terms (will be internally adjusted)
Kmin	15	-			min number of z-summation terms (will be internally adjusted)
Ncycles	20	-			max number of y-summation cycles
Kcycles	20	-			max number of z-summation cycles
cw	4180	J/M/K	J/kg/K		specific heat capacity of water (used for heat transport only)
cs	887	J/M/K	J/kg/K		specific heat capacity of solids (used for heat transport only)
Kw	0.64	W/L/K	W/m/K		thermal conductivity of water (used for heat transport only)
Ks	8	W/L/K	W/L/K		thermal conductivity of solids (used for heat transport only)
rhow	998	M/L^3	kg/m^3		density of water (used for heat transport only)
rhos	2.65	M/L^3	g/cm^3		density of solids
x	30	L		$0 \le x < \infty$ (Model1,3), $-\infty < x < \infty$ (Model 2, 4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3)	x-coordinate where output is computed
y	0	L		$0 \le y \le w$ (Model 1, 2, 3, 4), $-\infty < y < \infty$ (Model 4.1, 4.2, 4.3, 5.1, 5.2, 5.3)	y-coordinate where output is computed
z	100	L		$0 \le z \le b$	z-coordinate where output is computed
t	10	L		$t \ge 0$	time when output is computed
b	100	L		$b > 0$	aquifer thickness
w	100	L		$w > 0$	aquifer width
q	0.3	L/T		$q > 0$	Darcy flux
Sw	0.75	-		$0 \le Sw \le 1$	water saturation; default is 1; input only if different value is needed for unsaturated transport (without vapor phase)
theta	0.35	-		$0 \le theta \le 1$	water content (taken as porosity for saturated zone)
phi	0.5	-		$0 \le phi \le 1$	fraction of mobile porosity
f	0.5	-		$0 \le f \le 1$	fraction of mobile sorption sites
alpha	0.1	T^{-1}			transfer coefficient between mobile and immobile domain
lambdai	0.02	T^{-1}		$lambdai \ge 0$	first order decay for dissolved mass in immobile domain
lamdais	0.02	T^{-1}		$lamdais \ge 0$	first order decay for sorbed mass in immobile domain
lambdam	0.01	T^{-1}		$lambdam \ge 0$	first order decay for dissolved mass in mobile domain
lambdams	0.01	T^{-1}		$lambdams \ge 0$	first order decay for sorbed mass in mobile domain
gamma	0.8	-		$gamma > 0$	mass yield for parent to daughter product decay (ratio of molecular masses), only used by Model 3
Ki	0.1	L^3/M		$Ki \ge 0$	distribution coefficient for immobile domain

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All output instructions must be within block OUTPUT... ENDOUTPUT at the end of the file.
Units are shown as mass (M), length (L), time (T), energy (J), power (W), temperature (K)

Model input			*Units*	*Default Value Units*	*Allowed Value*	*Explanation*
Km	0.1		L^3/M		Km≥0	distribution coefficient for mobile domain
Dm	1.50E-09		L^2/T		Dm≥0	molecular diffusion coefficient in water
ax	100		L		ax≥0	dispersivity along x
ay	10		L		ay≥0	dispersivity along y
az	1		L		az≥0	dispersivity along z
x1	-10		L			source zone coordinate (starting x) used by Model 2 only
x2	0		L			source zone coordinate (ending x) used by Model 2 only
y1	0		L		0≤y1≤w	source zone coordinate (starting y)
y2	20		L		0≤y2≤w, y2>y1	source zone coordinate (ending y)
z1	80		L		0≤z1≤b	source zone coordinate (starting z)
z2	100		L		0≤z2≤b, z2>z1	source zone coordinate (ending z)
x0	10		L			point source coordinates used by Model 2 only; if all x0, y0, z0 are specified, Model 2 is evaluated for point source instead of volumetric source, otherwise they are ignored or x0, y0 used when injection=yes
y0	22		L		0≤y0≤w	
z0	50		L		0≤z0≤b	
h1	0.291		$W/L^2/K$		h1>0	heat transfer coefficient at bottom of aquifer (Model 5.1, 5.2, 5.3)
h2	0.308		$W/L^2/K$		h2>0	heat transfer coefficient at top of aquifer (Model 5.1, 5.2, 5.3)
r	10		L		r>0	radius of cylindircal zone with initial temperature/mass distribution (models 4.3, 5.3)
r0	0.05		L		r0>0	radius of casing for well injected with tracer (only used if injection = yes)
source	const				const, pulse, sine, exp, linear, line, step	source time-function; Model 1 and 2 can use all options; Model 3 can use all options for species 1 (and no source for daughter species) or constant, exp, pulse for all species (with different coefficients for each); models 4 and 4.1 only use pulse
injection	yes*				yes, no	instantaneous injection of tracer used for Models 2, 4, 4.1; source must be "pulse" (any input other than "yes" means "no")
V	1.5		L^3		V>0	injected volume (only used if injection = yes and source = pulse)
C0	1	mass transport	M/L^3 $M/L^3/T$		C0≥0	For Models 1 and 3, C0 is source concentration Cs. For Model 2 mass generation term M is given the value of C0. For Models 4, 4.1 and 4.2, C0 is initial concentration.
		heat transport	K W/L^3	K W/m^3		For Models 1, 4, and 5, C0 is the initial temparature change. For Model 2, C0 is the time-dependent heat generation rate per unit volume.
Cm0	20		M/L^3		Cm0≥0	For Model 2 with no source (source=pulse), initial concentration in mobile porosity (C0 is ignored)
Ci0	30		M/L^3		Ci0≥0	For Model 2 with no source (source=pulse), initial concentration in immobile porosity (C0 is ignored)
C1	0		M/L^3			source concentration used for line, sine
Cfile	sourceC.txt				(filename)	ASCII text file with source (time, concentration) data pairs, used by step or linear
lambdas	-0.01		T^{-1}			source decay used by exp
phis	1.2		rad			source phase used by sine
omegas	0.3		rad/T			source frequency used by sine

Table 1a
Input File Variable Explanation - Forward Execution

Explanation
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Comments, units, and variable explanations are in blue font.
Blank cells for allowed value mean numeric input.
Variable names in the first column are case-sensitive, numeric values in the second column are in free format. The space or tab separated pairs (name, value)
All output instructions must be within block OUTPUT... ENDOUTPUT at the end of the file.
Units are shown as mass (M), length (L), time (T), energy (J), power (W), temperature (K)

Model input		*Units*	*Default Value Units*	*Allowed Value*	*Explanation*
delta	0			0 or 1	0-first type, 1-thrid type source BC for Model 1 and 3
function	Cm			Cm, Ci, Mq, MD	Model computed variable: Cm = C mobile, Ci = C immobile, Mq = advective time-integrated mass flux (Model 1 only), MD = dispersive time-integrated mass flux (Model 1 only); use Cm for heat transport; default is C source. This line is legacy input for backward compatibility, GUI reads this variable inside the block OUTPUT.
type	steady*			steady, transient	default is transient (any other word than "steady" means transient simulation)
lambdai	0.01	T^{-1}			These variables must be specified for each species to run Model 3; the are repeated N-times for N species. They are read sequentially so each variable must be ordered to be assigned for the correct species. The values for lambda(m,i,s...), Ki, Km, gamma must not be the same for any two species (at least one variable must differ). If multiple sets are specified but Model 1 or 2 is executed, the first set of these variables is used. Gamma for parent species must be specified but is not used.
		T^{-1}			
lambdais	0.01				
lambdam	0.01	T^{-1}			
lambdams	0.01	T^{-1}			
gamma	1	-			
Ki	0.1	L^3/M			
Km	0.1	L^3/M			
C0	1	M/L^3			
OUTPUT					keyword, this block contains output instructions and must be at the end of the input file
output	t			t,x,y,z,xy,xz,yz,xyz	output is series, 2D grid, or 3D grid, as indicated; the specified coordinate is varied
function	Cm			Cm, Ci, Mq, MD	Model computed variable: C mobile, C immobile, advective time-integrated mass flux (Model 1 only), dispersive time-integrated mass flux (Model 1 only); use Cm for heat transport; default is C source.
Tstart	0	T		Tstart≥0	starting time
Tend	100	T			ending time
dT	1	T			time increment
Xstart	0	L		Xstart≥0 for Models 1 and 3, any value for Model 2	starting x
Xend	100	L			ending x
dX	1	L			x increment
Ystart	0	L		Ystart≥0	starting y
Yend	100	L		Yend≤w	ending y
dY	1	L			y increment
Zstart	0	L		Zstart≥0	starting z
Zend	100	L		Zend≤b	ending z
dZ	1	L			z increment
ENDOUTPUT					keyword

Table 1b
Input File Variable Explanation - Inverse Execution

Explanation
Input file is ASCII text.
Input file content is in the two columns below heading "Model input", in black font.
Comments, units, and variable explanations are in blue font.
Variable names are case-sensitive, numeric values are in free format. The space or tab separated pairs (name, value) may be in any order within each input block.
Units are shown as mass (M), length (L), time (T), energy (J), power (W), temperature (K)

<---	*Model input*	--->	*Units*	*Explanation*
INVERSE				beginning of inverse block, input for inverse execution
NOTE				
	this is an example input file for inverse execution			Descriptive note
ENDNOTE				
COEFFICIENTS				beginning of optional coefficient block
	TOL	1.00E-10	-	tolerance limit for Laplace transform
	Ntol	1.00E-03	-	tolerance limit for z-summation
	Ktol	1.00E-03	-	tolerance limit for y-summation
	Nmin	15	-	min number of y-summation terms
	Kmin	15	-	min number of z-summation terms
	Ncycles	10	-	max number of y-summation cycles
	Kcycles	10	-	max number of z-summation cycles
ENDCOEFFICIENTS				end of coefficient block
AQUIFER				beginning of aquifer block
	b	8.32	L	aquifer thickness
	w	50	L	aquifer width
	q	1.00E-06	L/T	Darcy flux
	theta	0.35		water content (taken as porosity for saturated zone)
	rhos	2650	M/L^3	density of solids
	phi	0.5	-	fraction of mobile porosity
	f	0.5	-	fraction of mobile sorption sites
	alpha	0.05	T^{-1}	transfer coefficient between mobile and immobile domain
	Dm	9.30E-08	L^2/T	molecular diffusion coefficient in water
	ax	1	L	dispersivity along x
	ay	0.1	L	dispersivity along y
	az	0.01	L	dispersivity along z
	lambdam	0	T^{-1}	first order decay for dissolved mass in mobile domain
	lambdams	0	T^{-1}	first order decay for sorbed mass in mobile domain
	lambdai	0	T^{-1}	first order decay for dissolved mass in immobile domain
	lambdais	0	T^{-1}	first order decay for sorbed mass in immobile domain
	gamma	1	-	mass yield for parent to daughter product decay, only used by Model 3
	Ki	0	L^3/M	distribution coefficient for immobile domain
	Km	0	L^3/M	distribution coefficient for mobile domain
	cw	4184	J/M/K	specific heat capacity of water (used for heat transport only)
	cs	1000	J/M/K	specific heat capacity of solids (used for heat transport only)
	Kw	0.598	W/L/K	thermal conductivity of water (used for heat transport only)
	Ks	8	W/L/K	thermal conductivity of solids (used for heat transport only)
	rhow	998	M/L^3	density of water (used for heat transport only)
ENDAQUIFER				end of aquifer block
TEST				beginning of test block
testname	FC951A1_T			test name
model		4.1		use Model 1, 2, 3, 4, 4.1, or 4.2
transport	heat			mass or heat transport
type		transient		steady or transient

injection	yes				if yes, model calculates extent of injected zone and heat exchange with aquifer
	SOURCE				beginning of source block
	source	pulse			source type (must be pulse for injection)
	V	0.378		L^3	injected volume
	r0	0.073165		L	well casing/screen radius
	x0	0		L	well x
	y0	25		L	well y
	z1	5.69		L	height of bottom of screen above aquifer bottom
	z2	8.32		L	height of top of screen above aquifer bottom
	C0	40		M/L^3	concentration or temperature of injected water
	step	0	9.5		first step (time, concentration/temperature)
	step	60000	5.1		second step; ignored if source=pulse
	step	120000	0		third step; ignored if source=pulse
	ENDSOURCE				end of source block
	OBSERVATIONS				beginning of observations block; there may be any number of observation blocks, one for each observation well
		obswellnam	FC951A1		observation well name (no spaces)
		index	0	-	index is only used for Model 3 observations to identify species
		x	0	L	well x
		y	25	L	well y
		z	7	L	well z
		stdv	0.1	same as C0	standard deviation of observations (used as weight)
		file	951A1-T_10.txt		name of ASCII file with observation data pairs (time, concentration/temperature)
	ENDOBSERVATIONS				end of observation block
ENDTEST					end of test block
TEST					
testname	FC951A1_C				
model		4.1			
transport	mass				
type		transient			
injection	yes				
	SOURCE				
	source	pulse			
	V	0.378		L^3	
	x0	0		L	
	y0	25		L	
	z1	5.69		L	
	z2	8.32		L	
	C0	19653		M/L^3	For Models 1 and 3, C0 is source concentration Cs. For Model 2 mass generation term M is given the value of C0. For Models 4 and 4.1, C0 is initial concentration.
	Cm0	19653		M/L^3	For Model 2 with no source, initial concentration in mobile porosity (C0 is ignored)
	Ci0	0		M/L^3	For Model 2 with no source, initial concentration in immobile porosity (C0 is ignored)
	step	0	1000		steps are ignored unless source = "step" or "linear" and model is 1,2,3
	step	60000	5000		
	step	120000	0		
	ENDSOURCE				
	OBSERVATIONS				
		obswellnam	FC951A1		
		index	0	-	index is only used for Model 3 observations to identify species
		x	0	L	
		y	25	L	

		z	7	L
		stdv	500	same as C0
		file	I51A1-C_10.txt	
	ENDOBSERVATIONS			
ENDTEST				
GENETIC				beginning of genetic algorithm instructions
	Ngenerations	10		number of generations (not including initial, starting generation)
	Nchromosomes	99		number of chromosomes (individual solutions)
	Ntournament	3		number of chromosomes used in tournament selection
	keepsurvivors	yes	yes, no	keep selection survivors in next generation, or replace all
	*alpha	0.1		factor controling objective function parts (disabled by adding any character)
	mutation	0.05		mutation probability for offspring
ENDGENETIC				end of genetic algorithm instructions
MCMH				beginning of Markov chain Monte Carlo instructions
	N	1000		number of steps in one chain (chain length)
	Nchain	3		number of consecutive chains
	Nb	100		lenbgth of burn-in (before first chain)
	Gibbs	no	yes, no	Gibbs sampling or not (sequential application of Metropolis criterion for every individual parameter within each chain step)
	restart	no	yes, no	restart from random initial guesses (ignore GA results)
	*alpha	0		factor controling objective function parts (disabled by adding any character)
	Nhist	50		number of bins for output histograms
ENDMCMH				end of Markov chain Monte Carlo instructions
PARAMETER				beginning of parameter block
	name	q		parameter name (must be one of input variable names)
	index	0		index is only used for Model 3 parameters for chain decay
	distribution	G	G, U, T	Gaussian (G), uniform (U), or triangular distribution (T) is used to draw new values
	log	yes	yes, no	operate on natural logarithm of parameter value
	prior	1.00E-06		prior parameter value, used in parameter constraint portion of objective function (should be determined independently of the test being analyzed); if not defined, prior = ini
	ini	1.00E-06		initial value
	stdv	5		parameter standard deviation used as weighting factor in objective function, applies to prior value; note this is for a log-normal distribution
	min	1.00E-10		minimum allowed value
	max	1.00E-01		maximum allowed value
	cv	0.01		parameter coefficient of variation used in calculation of random values from current parameter value (that's why a fractional number is specified)
ENDPARAMETER				
PARAMETER***				disabled parameter block; ignored
	name	alpha		
	index	0		
	distribution	G		
	log	yes		
	prior	1.00E-02		
	ini	1.00E-02		
	stdv	3		
	min	1.00E-08		
	max	0.1		
	cv	0.01		
ENDPARAMETER				

```
PARAMETER
        name            theta
        index           0
        distribution    G
        log             yes
        prior           0.3
        ini             0.35
        stdv            2
        min             1.00E-03
        max             0.6
        cv              0.01
ENDPARAMETER

PARAMETER
        name            ax
        index           0
        distribution    G
        log             yes
        prior           1
        ini             1
        stdv            2
        min             1.00E-05
        max             100
        cv              0.01
ENDPARAMETER

TIEDPARAMETER                                   beginning of tied parameter block
        name            ay                      parameter name (must be one of input variable names)
        index           0                       index is only used for Model 3 parameters for chain decay
        master          ax                      master parameter to which this parameter is tied to
        masterindex     0                       index is only used for Model 3 parameters for chain decay
        multiplier      0.1                     multiplying factor: Ptied = multiplier * Pmaster + offset
        offset          0                       offset: Ptied = multiplier * Pmaster + offset
ENDTIEDPARAMETER                                end of tied parameter block

TIEDPARAMETER
        name            az
        index           0
        master          ax
        masterindex     0
        multiplier      0.01
        offset          0
ENDTIEDPARAMETER


ENDINVERSE                                      end of instructions for inverse execution
```

Table 2
Source Types for Models

Source Time Dependence	Explanation	Model Using Source Type
const	Constant in time	1, 2, 3
pulse	Instantaneous pulse	1, 2, 3
sine	Sinusoidal oscillation plus constant	1, 2, 3 (first species only)
exp	Exponential increase or decrease	1, 2, 3
line	Linear trend	1, 2, 3 (first species only)
step	Constant step changes at multiple points	1, 2, 3 (first species only)
linear	Linear interpolation between multiple points	1, 2, 3 (first species only)
no source	Initial concentration/temperature distribution	2, 4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3

Notes

shifted sine	$C_s(t) = C_0 + C_1 \sin(w_s t - \varphi_s)$	The constant C0 is to avoid negative values.
line	$C_s(t) = a_0 + a_1 t$	(C0 and C1 are used for a0 and a1)
exponential	$C_s(t) = C_0 \exp(\lambda_s t)$	

Source geometry is:

- Vertical rectangle with time-dependent type 1 or 3 BC (Model 1, 3)
- Rectangular prism with time-dependent mass/heat generation (Model 2)
- Rectangular prism with initial concentration/temperature (Model 2, 4, 4.1, 5.1)
- Gaussian cylinder with initial concentration/temperature (Model 4.2, 5.2)
- Cylinder with initial concentration/temperature (Model 4.3, 5.3)

Linear trend (line) source is truncated at zero if specified as decreasing to avoid negative values.

Step and linear source types use a set of time, concentration (or mass rate) data pairs supplied in a separate input file.

All species have the same source type in Model 3 for pulse, const, exp but each has different coefficients.

When the source is sine, step, linear, or line for the first species in Model 3, the daughter species have zero source.

If heat transport is simulated and pulse is selected for Model 2, the input is initial equilibrium temperature.

Table 3
Source Options for Models

	Source option		
Model	**Transient**		**Steady**
1	all		const
2	all	if source=pulse, Cm0, Ci0 must be unspecified (do not include in input file)	const
	none	Ci0, Cm0 are initial concentrations	NA
	sine, line, step, linear for Species 1	no source for daughter species	NA
3	const, pulse, exp for all species	same source type for all species (C0 and lamdas may differ for each species)	const
4, 4.1, 4.2, 4.3	none	C0 is the initial concentration (temperature)	NA
5.1, 5.2, 5.3	none	C0 is the initial concentration (temperature)	NA

Injection
Only for Model 2, 4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3
Only transient
V, r0, x0, y0 must be given values
z1,z2 must be given values

Heat Transport
Only Model 1, 2, 4, 4.1, 4.2, 4.3, 5.1, 5.2, 5.3

Table 4
Example Values for Selected Variables

Variable	*Value*	*Units*	*Note*	*Explanation*
cw	4180	J/kg/K	water	specific heat capacity of water (used for heat transport only)
cs	887	J/kg/K	quartz, feldspars	specific heat capacity of solids (used for heat transport only)
Kw	0.64	W/m/K	water	thermal conductivity of water (used for heat transport only)
Ks	8	W/m/K	quartz, feldspars	thermal conductivity of solids (used for heat transport only)
rhow	998	kg/m^3	water	density of water (used for heat transport only)
rhos	2650	kg/m^3	quartz	density of solids
Sw	1	-	0≤Sw≤1	water saturation; default is 1; input only if different value is needed for unsaturated transport
theta	0.3 - 0.5	-	0≤theta≤1	water content (taken as porosity for saturated zone)
phi	0.5	-	0≤phi≤1	fraction of mobile porosity
f	0.5	-	0≤f≤1	fraction of mobile sorption sites
alpha	1.00E-05	s^{-1}		transfer coefficient between mobile and immobile domain
lambdam	1.90E-03	d^{-1}	lambdam≥0	first order decay for dissolved mass in mobile domain corresponding to a half-life of 1 year
lambdam	2.198E-08	s^{-1}	lambdam≥0	first order decay for dissolved mass in mobile domain corresponding to a half-life of 1 year
Ki	0.01	m^3/kg	TCE	distribution coefficient for immobile domain, K = KOC*foc, KOC = 101 m^3/kg, foc = 1.0e-4
Km	0.01	m^3/kg	TCE	distribution coefficient for mobile domain, K = KOC*foc, KOC = 101 m3/kg, foc = 1.0e-4
Dm	1E-09	m^2/s	TCE in water	molecular diffusion coefficient in water
Dm	1.50E-09	m^2/s	NaCl in water	molecular diffusion coefficient in water
ax	1	m	ax≥0	dispersivity along x
ay	0.1	m	ay≥0	dispersivity along y
az	0.01	m	az≥0	dispersivity along z
q	1.00E-06	m/s	a≥0	Darcy flux along x; q = K*i