A short tutorial how to implement a PHREEQC 1d transport and ion exchange reaction example in ORCHESTRA

Hans Meeussen 26/11/2024

This document describes how implement a simple PHREEQC ion exchange and 1d transport example in ORCHESTRA. The example was taken from the very useful PHREEQC site by Tony Appelo and the PHREEQC description can be found here:

Chromatographic displacement of ions (hydrochemistry.eu)

The example demonstrates how to calculate the composition of a chromatographic column that is first in equilibrated with 1 mmol NaNO₃ plus 0.2 mmol KNO₃ and subsequently flushed with a 0.6 mmol CaCl₂ solution. This results in the following concentration breakthrough pattern at the outflow:



The definition of the PHREEQC initial condition of input and column solution is, as always, very compact. We can see here the composition of both solutions, including the 0.0011 mol of exchanger surface present.

TITLE Example 11.--Transport and cation exchange. SOLUTION 0 CaCl2 units mmol/kgw

temp 25.0 рΗ 7.0 charge 12.5 02(g) -0.68 ре Са 0.6 1.2 Cl SOLUTION 1-40 Initial solution for column mmol/kgw units 25.0 temp 7.0 рΗ charge 02(g) -0.68 ре 12.5 Na 1.0 0.2 Κ N(5) 1.2 END EXCHANGE 1-40 -equilibrate 1 Х 0.0011 COPY cell 1 101 END

This is short description is very elegant, but to reproduce it with another code it is necessary to understand what is going on behind the screen!

ORCHESTRA implementation

The definition of all the required system parts and calculation tasks can be found in the concert.xml file. A screenshot is shown here, but the complete file is present in the accompanying folder.

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To define the same system in ORCHESTRA, we need the same 40 cells for the transport system (cell1-40), plus a cell that represents the input solution (cell 0) and another one that represents a waste bucket (cell 41) that will be used as a sink at the end of the column. We actually define 42 cells.

In the concert file a number of different calculation or input output tasks are defined, and at the bottom the "Run" task contains the tasks that are carried out during a run.

Here we can see that the system is first initialized by reading the composition of cells 0-40 from an input file, and subsequently for each of these cells a solver (chemistry1.inp) is used to calculate the initial chemical composition.

We need two solvers in this system; one to calculate the initial composition of the system with given dissolved concentrations as input (<name>.diss), and a second calculator that is used during transport that uses the given total amount of substances (<name>.tot) in a cell as input.

So these solvers only differ in the definition of the primary entities / master species:

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chemistry1.inp					Read			Write				GUI V	ïew		Intro Descrip	tion
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E tot	t pe		V	-7.0			E.I	logact = -pe		_						
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🖌 Na tot	t				0.1	diss										
✓ O tot	t H2	O.logact	V	0.0			0.	logact = H2O.logact								
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tot diss min gas					Include		C	Database				advection
P A Acetate					V	minteq.v4.dat						dispersion
S B Ag					V	adsorption.txt						concert
T C AI												feed
U D Alkalinity												column
V E As												outputsolution
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Selected Primary Entit	ies/ Master S	pecies								Add c	latabase file	
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Ca tot			1.08	-9 tot		Expression						
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E tot	pe	-7	.0		E.I	ogact = -pe		_				
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Both solvers contain the same set of chemical reactions (including ion exchange reactions):

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Phase Hierarchy and Entities										initial_solid_composition
Reactions in all phases										chemistry1
← □ tot (1)	Formation reacti	ons in phase: all	, depending	g on primary entity:	all 🔻 and: all 💌	Hide	unselected 🔲 🖊	Alphabetical 🗹	Select all list	chemistry2
P Iter (watervolume										advection
solution (1)	Incl.	Name	Lo	g K (25C)	Phase		Coef.	Reactant	Coe	dispersion
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e 🗖 colloid (1)	CaNO3+		5.000000e-1		diss	1	.0 Ca+2		1.0	feed
			-12.69700		diee				-1.0	column
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	Exch X-K		7.00000e-1		Exch X	1	.0 Exch X		1.0	outputprofile
	Exch_X-Na		0.0		Exch_X	1	.0 Exch_X		1.0	
	Exch_X2-Ca		8.00000e-1		Exch_X	1	.0 Ca+2		2.0	
	✓ H+		0.0		diss	1	.0 H[+1]			
min (1)	✓ H2		0.0		diss	1	.0 H[+0]			
• ads (1)	H2O		0.0		liter	1	.0 0[-2]		2.0	
P CLAY_P			-3.150000		tot	4	0 4		2.0	
			-1.602500		min		0 Ch		1.0	
P 📑 HFO_pa -	K+		0.0		diss		.0 K			
HFC -	Lime[s]		-32.69930		min	1	.0 Ca+2		-2.0	
💡 📑 Goethite	NO3-		0.0		diss	1	.0 N[+5]			
- 🗋 Goe	N[+3]		28.57000		tot	4	2.0 H+		-1.0	
🕈 📑 SHA_pa	✓ N[+5]		0.0		tot	1	.0 N			
	N[-3]		1.190770e2		tot	1	0.0 H+		-3.0	
SFA pa	Na+		0.0		diss	1	.0 Na			
	V NaUH		-14.18000		diss	-	1.0 H+		1.0	
e E Eych	02[a]		-83 08940		0155		4.0 H+		2.0	
	V OH-		-13,99950		diss	-	1.0 H+		1.0	
	[0+10 V		-85,99508		tot	-	4.0 H+		2.0	
Y gas_1 (1)	✓ O[-2]		0.0		tot	1	.0 O			
gas ((gas)	Portlandite[s		-22.80400		min	1	.0 Ca+2		-2.0	
Y (1)	✓ e-		0.0		diss	1	.0 E			
P litter (1/SL)										
solution (1)	4									
	-									
to input file or directory selected.										

And the same amount of exchange surface (1.1e-3 mol/l)

				I	1	4	Intro
chemistry2	2.inp		Read	Write	GUI View		Description
Extra Taxt	Adsorption models Activ	ity correction		n Output selector			parameters
Exua lext	Primary entit	ties/ Master Specie		Phases & Reactions	Var	riables	initial_solid_composition
	Fillinary enu	lies/ master specie	55	Filases & Reactions	vai	lables	chemistry1
	Edge						chemistry2
		Includes 🗖 No.	www.Edual Descent Destining and				advection
		Include: Na	ime: Edge Parent Particle: surto	Specific surface area m2/kg: 16	e-3		dispersion
							concert
							feed
							column
							outputsolution
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	Exch						
		Include: 🗹 Nan	me: Exch Parent Particle: ads	Specific surface area m2/kg: 1.1	e-3		
	//The PHREEQC EXCHANGE_MA: Exch Exch-	definition for compa	arison				

In contrast with PHREEQC, in the ORCHESTRA input file all (adsorption) reactions are present and copied from the database(s). So the databases are only used when the system is interactively defined, and not required during a run.

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cnemistry2.inp			Read		Write				GUI View		Description
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Phase Hierarchy and Entities											initial_solid_compositio
Reactions is all phases											chemistry1
Contractions in all phases	Formati	ion reactions in phase:	all 🔽	, depending on p	rimary entity:	all 🔻 and: all 👻 H	ide unsele	ted 🔲 Alphabetical 🖌	Select all liste	d Select all recur	chemistry2
											advection
P inter (watervolume)	Incl.	Name		Log K (2	5C)	Phase	Coef.	Reactant	Coef.	Reactar	dispersion
Solution (1)	Ca+	+2	0	.0	/	diss	1.0	Ca			concert
- diss (1)	CaN	NO3+	5	.000000e-1		diss	1.0	Ca+2	1.0	NO3-	feed
colloid (1)	CaC	CH+	-1	2.69700		diss	1.0	Ca+2	-1.0	H+	column
DHA_part (1)	CI-		0	.0		diss	1.0	CI			outputsolution
HA_part (DHA_kgl)	Excl	h_X-H	1	.000000		Exch_X	1.0	Exch_X	1.0	H+	ouputsolution
P □ DFA_part (1)	Excl	h_X-K	7	.000000e-1		Exch_X	1.0	Exch_X	1.0	K+	outputprofile
FA part (DFA kol)	Excl	h_X-Na	0	.0		Exch_X	1.0	Exch_X	1.0	Na+	
solid (1)	Excl	h_X2-Ca	8	.000000e-1		Exch_X	1.0	Ca+2	2.0	Exch_X	
	H+		0	.0		diss	1.0	H[+1]			
	HZ HZ		0	.0		diss	1.0	H[+U]			
9 ads (1)	HZC HZC	01	0	150000		liter	1.0	0[-2]	2.0	- 1	
CLAY_part_I (1)		41	-3	.150000		tot	2.0	H	2.0	e-	
CLAY_part (CLAY_kgkg		i la la la	1	802500		tot	1.0		1.0	Mai	
P [HFO_part_I (1)		(als)	- 1	0		diag	1.0		1.0	INGT	
HFO_part (HFO_kgkg*S	Lim	مادا	-3	2 69930		min	1.0	Ca+2	-2.0	Ha	
Goethite part (1)	NO:	3-		0		diss	1.0	N[+5]	-2.0		
Goethite part (Goethite	NI+:	31	2	8.57000		tot	2.0	H+	-1.0	H2O	
CE CHA and L (0)	V NI+	51	0	0		tot	1.0	N	- 1.0		
Y STA_part_1 (1)	NI-3	31	1	190770e2		tot	10.0	H+	-3.0	H2O	
MA_part (SHA_kgkg*SL)	Na+		0	0		diss	1.0	Na			
SFA_part_I (1)	NaC	ЭН	-1	4.18000		diss	-1.0	H+	1.0	H2O	
FA_part (SFA_kgkg*SL)	✓ 02		0	.0		diss	1.0	O[+0]			
Exch (1.1e-3)	02	[g]	-8	3.08940		gas	-4.0	H+	2.0	H2O	
Exch X (1)	CH-		-1	3.99950		diss	-1.0	H+	1.0	H2O	
a a a a a a a a a a a a a a a a a a a	V 0[+	0]	-8	5.99508		tot	-4.0	H+	2.0	0	
	PI OI-	21	0	0		tot	10	0		×	
	•										
o input file or directory selected	_						_				H.

In case of adsorption models, the complete model definition is also copied to the input file. So not only the adsorption reactions, but also the underlying adsorption model code. In case of ion exchange model, this is only a very limited amount of code. Switching to text representation of the GUI View makes this visible.

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-				parameters		
//**** Model type code **	**			initial_solid_composition		
@class: adsorptionmodelco	de(Basic surface){			chemistry1		
@class: Basic surface(chemistry2					
// The Basic surfac	e model just contains of	a single phase		advection		
<pre>// that is linked t</pre>	o its parent phase via it	s concentration		dispersion		
<pre>@phase(<name>, <par< pre=""></par<></name></pre>	ent_phase>, <concentratio< th=""><th>n>)</th><th></th><td>concert</td></concentratio<>	n>)		concert		
}				feed		
3				column		
@adsorptionmodelcode(Basi	c_surface)			outputsolution		
//**** End of model type	code ****			outputprofile		
@adsmodel(Exch, ads ,1.1e	-3, Basic_surface)					
<pre>@surfsite(Exch, X, 1, 0)</pre>						
@surfspecies(Exch, X, X-H	, 1)					
<pre>@logKreaction(Exch_X-H, 1</pre>	.0, 1.0, Exch_X, 1.0, H+)					
@surfspecies(Exch, X, X-K	, 1)					
<pre>@logKreaction(Exch_X-K, 0</pre>	.7, 1.0, Exch_X, 1.0, K+)					
dsurfspecies (Exch, X, X-N	a, 1)					
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esurispecies (Exch, X, X2-	Ca, 0.5)	5. ar.)	=			
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Definition of chemical input parameters in parameter file

We now have our chemical model defined in the two chemical calculators, and next we can give the values for the initial concentrations in the input file and column. The values are given in the parameter.txt file. Here you find the definition of 41 compositions (for the input solution, cell 0 + 40 column cells). In this case this definition is stored in a "class" chemical_cell_parameters, that is used in the "initial_solid_composition" input file.

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parameters.t	xt		Read Write lext View									Description
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//**** define	chemical parame	ters for 41	cells.	used	l in initia	l solid com	position.da	t				initial_solid_composition
<pre>@class: chemical_cell_parameters() (</pre>												chemistry1
CARDA CHARTONY FRAME OF A CAL											chemistry2	
// the first :	line of data poi	nts defines	the in	put s	olution (c	ell 0)						advection
// note that	this cell is cal	culated wit	h chemi	stry	1, so amou	nts in mol/	liter as in	put				dispersion
// note that (ix represents ha	lf the cell	thickn	aess (distance f	rom cell ce	ntre to bou	indary)				concert
Var: to	tvolume dx	porosity	pн	pe	Na.diss	K.diss	N.diss	Cl.diss	Ca.dis	s		feed
Data:	L 0.001	1	7	7	1e-9	1e-9	1e-9	1.2e-3	6e-4			column
												outputsolution
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<pre>// The follow: // these cell:</pre>	ing datalines de s is initialized	fine the in with chemi	itial c stry 1	amoun	ition of t ts in mol	he column m liter	aterial					
Var: to	tvolume dx	porosity	pн	pe	Na.diss	K.diss	N.diss	Cl.diss	Ca.diss			
Default: 1	0.00	1 1	7	7	1e-3	0.2e-3	1.2e-3	1e-9	1e-9			
											=	
// 40 cells												
Sweep: 40												
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				chemistry1
				chemistry2
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No input file or directory colocted			·	9

By clicking on text view you can check that the @chemical_cell_parameters() statement is correctly expanded to the full text in the parameters file.

This expanded text is used as input, as all input files are by default expanded.

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Var: totvolume dx Default: 1 0.0 Sweep{ 40	porosity pH pe Na.diss 01 1 7 7 1e-3	K.diss N.diss Cl.dis 0.2e-3 1.2e-3 1e	s Ca.diss -9 le-9	concert feed column outputsolution outputprofile			
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The parameter file also contains several transport parameters

📓 ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores) - D X									
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paramotors tyt	Boad	Write	Taxt View	1	I	ntro			
parameters.txt	Reau	Wille	Text view		Description				
					para	meters			
<pre>@def: totaltime(){25} //hou</pre>	initial_solid	I_compo	osition						
<pre>@def: timestep() {100} //s</pre>	ecs				che	mistry1			
<pre>@def: nrtimesteps(){@evalua</pre>	te:("@totaltime()*3600/@tim	estep()")}			che	mistry2			
<pre>@def: tortuosity() { @evalu</pre>	<pre>ate:("sqrt(10)")} // only</pre>	important for diffusion			adv	rection]		
					disr	persion]		
<pre>// Here we calculate the fl</pre>	ow rate that we select in s	uch a way that we get .1 po:	revolume per hour	=	co	ncert			
<pre>// we have 50 cells of 1 li</pre>	ter so total porevolume = 4	0 liter			f	feed			
<pre>// however we get output fo</pre>	or the centre of the last ce	ll, which is half a			CC	column			
<pre>// cell earlier, so total p</pre>	orevolume equals 39.5 liter	and 0.1 porevolume 3.95 li	ter.		outpu	tsolution	<u>n</u>		
<pre>// (This is similar to the</pre>	description of PHREEQC)				outpr	utprofile	,		
<pre>@def: flowrate(){@evaluate:</pre>	("3.95/3600")} // liter per	sec							
// 1 PV of complete column	= 40 liter								
// 0.1 pv/hour = 4/3600 lit	er per second, so output un	its 1 hr = 1 pv							
// Numerical dispersion in	this column for unretarded	front							
// dx/2 - Vdt/2R									
evaluate: ("(0.002/2)-((3.9									
// so the numerical dispers									
// so the numerical dispers	sporsivity to obtain 20-3 m	in total							
def: dispersivity() (1 11e-	apersivity to obtain 20-3 M	in cotal.							
eact. arspersivity () {1.11e-									
No input file or directory selected					1				

Which are mainly used in the feed.dat file:

Subscription of Weight Street		- 🗆 X		
<u>File Run T</u> ools <u>H</u> elp				
fer and shake				Intro
reed.dat	Read	Write	Text View	Description
@include: parameters.txt			▲	parameters
				initial_solid_composition
Var: dt J				chemistry1
Default: 1 @flows	rate()			chemistry2
				advection
Sweep: @nrtimesteps()				dispersion
Swept: dt @timestep() @tim	mestep() lin			concert
}				feed
				column
				outputsolution
				outputprofile
			•	
2 Na investila en dina stanta a la stant				1

No input file or directory selected.

Which is also expanded at read in time:

legional ORCHESTRA-Composer (Running on W	- 🗆 X						
File Run Tools Help							
Construction (Intro			
reed.dat	Read	Write	Expanded View	Description			
Var: dt J		·		parameters			
Default: 1 1.097	/22e-3			initial_solid_composition			
				chemistry1			
Sweep: 9.00000e2				chemistry2			
Swept: dt 100 100 lin				advection			
}				dispersion			
				concert			
				feed			
				column			
				outputsolution			
				outputprofile			
No input file or directory selected.							

And contains the timestep (100 sec), total number of timesteps (900) and flow speed (liter / sec).

Definition output variables and frequency in output file

The system has two different output files

- 1) Outputsolution.dat that contains the composition of the last cell and is called every timestep
- 2) Outputprofile.dat that contains the composition of all cells

In the concert file these two files are defined as follows:

Superior Context Conte								\times
<u>File Run T</u> ools <u>H</u> elp	File Run Tools Help							
Intro							utsolutio	n
concert.xml	Read	Write	Text View		Description	out	outprofile	, ``
<task name="Write outp</td><td>out profile" type="Outstre</td><td>amGroup"></task>		-	parameters					
<file>output profil</file>	.e.dat	-			initial_solid_composition			
<nodes>(0-40)<td>s></td><td></td><td></td><td></td><td>chemistry1</td><td></td><td></td><td></td></nodes>	s>				chemistry1			
					chemistry2			
					advection			
<task name="Write outp</td><td>out_solution" type="Outstr</td><td>reamGroup"></task>			dispersion					
<file>output_solution.dat</file>					concert			
<nodes>(40)</nodes>					feed			
(/Idsk/				•	column			
No input file or directory selected.					1			

And called every timestep:

GRCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores)							
<u>File Run T</u> ools <u>H</u> elp	File Run Tools Help						
				Intro			
concert.xml	Read	Write	Text View	Description			
				parameters			
<pre>/maak Nama="Fach Mimoston" "</pre>	mo-"Poposting Tack (noun ")			initial_solid_composition			
Chomask Name="Bead feed no	de" />			chemistry1			
<pre>Collast Name= Read leed in Collast Name="Equilibrate</pre>	<pre>cbordsk Name="kead leed node" /> cbordsk Name="kead leed node" /></pre>						
<dotask name="Equilibrate</td><th>all nodes 2"></dotask> <th></th> <th></th> <td>advection</td>			advection				
<dotask name="Write output</td><th>t profile"></dotask> <th></th> <th></th> <td>dispersion</td>			dispersion				
<pre><dotask name="Write output</pre></td><th>t solution"></dotask><th></th><th></th><td>concert</td></pre>			concert				
<dotask name="Calculate ad</td><th>
ivection"></dotask> <th></th> <th></th> <td>feed</td>			feed				
<dotask name="Calculate d:</td><th>ispersion"></dotask> <th></th> <th></th> <td>column</td>			column				
<dotask name="Clock update"></dotask>				outputsolution			
<dotask name="View"></dotask>							
// <dotask name="Wait"></dotask>							
· · · · · · · · · · · · · · · · · · ·			<u> </u>				

The content and frequency of the output is defined within the output file. So for output solution we get output for the listed variables every 0.1 hour from 0 to 25 hours.

a ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores)											
File Run Tools Help											
			1		Intro						
output	_solution.dat	Read	Write	Text View	Description						
Output	at: (time hours, from:, 0, to	:, 25, step:, .1)			parameters						
// The	column headers in this file ca	an be edited and determine the output	t for the next run.		initial_solid_composition						
Var:	time hours	Na.diss	K.diss	Ca.diss Cl.di	ss chemistry1						
Data:	0.0	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	chemistry2						
Data:	1.11111111e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	o advection						
Data:	2.2222222e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	o dispersion						
Data:	3.05555556e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	0 concert						
Data:	4.16666667e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00 feed						
Data:	5.0000000e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	o column						
Data:	6.11111111e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00 outputsolution						
Data:	7.22222222e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	0 outputprofile						
Data:	8.05555556e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	9.16666667e-1	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	1.0000000	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	1.11111111	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	1.22222222	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	30						
Data:	1.30555556	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	1.41666667	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	1.5000000	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	30						
Data:	1.61111111	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	00						
Data:	1.72222222	1.0000000e-3	2.0000000e-4	1.0000000e-9 1.000	20-						
		m			<u></u>						
No input f	ile or directory selected.			o input file or directory selected.							

For output of the complete profile we specify the times at which we want output:

ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Orade Corporation, using 24 processing cores)								
Eile Rur	File Run Tools Help							
						Intro		
output	_profile.dat	Read		Write	Text View	Description		
Output	at: (time hours, 0, 1, 2, 5, 10,	25)				parameters		
// The	column headers in this file can	be edited and determine	the output for	the next run.		initial_solid_composition		
Var:	time hours	Node ID	- J	рН	Ca.diss	chemistry1		
Data:	0.0	0.0	0.0	7.0000000	6.0000000e-4	chemistry2		
Data:	0.0	1.0000000	0.0	7.0000000	1.0000000e-9	advection		
Data:	0.0	2.0000000	0.0	7.0000000	1.0000000e-9	dispersion		
Data:	0.0	3.0000000	0.0	7.0000000	1.0000000e-9	concert		
Data:	0.0	4.0000000	0.0	7.0000000	1.0000000e-9	feed		
Data:	0.0	5.0000000	0.0	7.0000000	1.0000000e-9	column		
Data:	0.0	6.0000000	0.0	7.0000000	1.0000000e-9	outputsolution		
Data:	0.0	7.0000000	0.0	7.0000000	1.0000000e-9	outputprofile		
Data:	0.0	8.0000000	0.0	7.0000000	1.0000000e-9	(
Data:	0.0	9.0000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	10.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	11.0000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	12.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	13.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	14.0000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	15.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	16.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	17.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	18.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	19.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	20.000000	0.0	7.0000000	1.0000000e-9			
Data:	0.0	21.0000000	0.0	7.0000000	1.0000000e-9 👻			
•		Н						

No input file or directory selected.

So please note that output times and output variables are defined within the output files themselves!!

Definition of Advection and Dispersion

In the concert.xml file you will also find two transport tasks defined; advection and dispersion.

These tasks are defined as a set of connections of links between cells. For each of these connections some calculations are defined in the advection.inp and dispersion.inp text files.

Note that the connections for the advection and dispersion task are not exactly the same: the dispersion task does not have the connection with the final node 41 (waste bucket or sink).

This waste bucket is only used by advection to remove all mass that leaves cell 40. Advection does not look at the content of cell 41, so cell 41 does not contain realistic concentrations (is not calculated or updated). However, dispersion (like diffusion) is a function of the concentrations in the two connected cells, so in this case the (unrealistic) concentrations in cell 41, would result in errors. (you can try this for yourself by adding the link 40-41 and check the results.



Calculation of advection and dispersion happens every timestep (after all nodes/cells are equilibrated).

ORCHESTRA-Composer (Running or)	- 🗆	\times				
<u>File Run</u> Tools Help						
	Intro					
concert.xml	Description					
<dotask name="Update</td><td>parameters</td><td>]</td></tr><tr><td></Task></td><th></th><td></td><td></td><td>initial_solid_composit</td><td>ion</td></tr><tr><td></td><th></th><td></td><td></td><td>chemistry1</td><td>]</td></tr><tr><td><Task Name=" time="</td><th>'200" type="WaitTask" wait"=""> <td>k></td><td></td><td>chemistry2</td><td></td></dotask>	k>		chemistry2			
				advection		
<task name="Each Timeste</td><th>p" type="RepeatingTaskGroup</th><td>"></task>		dispersion				
<dotask name="Read fe</td><th>ed node"></dotask> <td></td> <td></td> <td>concert</td> <td></td>			concert			
<dotask name="Equilib</td><th>orate node 0"></dotask> <td></td> <td></td> <td>feed</td> <td></td>			feed			
<dotask name="Equilib</td><th>orate all nodes 2"></dotask> <td></td> <td></td> <td>column</td> <td></td>			column			
<dotask name="Write o</td><th>output_profile"></dotask> <td></td> <td></td> <td>outputsolution</td> <td></td>			outputsolution			
<dotask name="Write o</td><th>output_solution"></dotask> <td></td> <td></td> <td>outputprofile</td> <td></td>			outputprofile			
<dotask name="Calcula</td><th>ate advection"></dotask> <td></td> <td></td> <td></td> <td></td>						
<dotask name="Calcula</td><th>ate dispersion"></dotask> <td></td> <td></td> <td></td> <td></td>						
<dotask name="Clock_u</td><th>update"></dotask> <td></td> <td></td> <td></td> <td></td>						
<dotask <="" name="View" td=""><th>/></th><td></td><td>1</td><td></td><td></td></dotask>	/>		1			
// <dotask name="Wait"></dotask>						
			-	•		
No input file or directory selected	-			-		

The actual calculations that take place for advection and dispersion are defined in the advection.inp and dispersion.inp input files.

Here a class "advec" is defined that calculates the mass transport (calculates delta masses in both connected cells) using the amount of water and the concentration of the incoming solution as input.

This advec class is called of each primary entity / master species.

▲ ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores)					\times			
<u>File Run T</u> ools <u>H</u> elp								
a dua stisus in a	_ .			Intro				
advection.inp	Read	Write	Text View	Description]			
@include: parameters.txt				parameters]			
-				initial_solid_composit	ition			
@Class: water flow()				chemistry1]			
This object contains the ger	chemistry2							
amount of water transported	amount of water transported between cell 1 and cell 2.							
It should be used in convect	tion.inp before the componen	it specific objects.		dispersion				
{ @Var: dwater 0				concert				
@Var: 1.J 0				feed				
				column				
//The amount of water mov	ving from cell 1 to cell 2 e	equals the		outputsolution				
<pre>//flow rate (l/s).</pre>				outputprofile				
<pre>@Calc:(1, "dwater = 1.J")</pre>	1							
}								
<pre>@Class: advec (name)</pre>								
This object contains the con	aponent specific part of con	vection and defines the						
amount of component (mol/s)	transported between cell 1	and cell 2.						
{ @globalvar: 1. <name>.solu</name>	ition 0							
@globalvar: 2. <name>.solu</name>	ition 0							
@Var: 1. <name>.d 0</name>				=				
@Var: 2. <name>.d 0</name>								
@Var: dmass 0								
//Calculate the transport	ted mass between cell 1 and	cell 2						
//depending on the direct	tion of the flow							
<pre>@Calc:(1, "dmass = dwater</pre>	r * if (dwater>0 . {1. <name></name>	<pre>.solution}. {2.<name>.soluti</name></pre>	(on})")					
$(Calc: (1, "1, $	(
@Calc: (1, "2. <name>.d = {2</name>	$2..d} + dmass")$							
}								
<pre>@class: component(name) {</pre>								
@advec(<name>)</name>								
}								
@water_flow()								
<pre>// This automatically include</pre>	ies advection for all select	ed components						
@include: chemistry1_compone	ents.inp							
<u></u>								
No input file or directory selected.								

You can check this by clicking on the "Text view button"

🗟 ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores) - 🗆 🗙					
<u>F</u> ile <u>R</u> un <u>T</u> ools <u>H</u> elp					
advaction inn	Poad	Write	Expanded View	Intro	
advection.inp	Reau	WITCH	Expanded view	Description	
@Var: dwater 0			▲	parameters	
@Var: 1.J 0				initial_solid_composition	
				chemistry1	
				chemistry2	
				advection	
<pre>@Calc:(1, "dwater = 1.J")</pre>				dispersion	
				concert	
// This automatically includ	les advection for all selecte	ed components		feed	
@globalvar: 1.Ca.solution 0				column	
<pre>@globalvar: 2.Ca.solution</pre>	1 0			outputsolution	
@Var: 1.Ca.d 0				outputprofile	
@Var: 2.Ca.d 0			=		
@Var: dmass 0					
<pre>@Calc:(1, "dmass = dwater</pre>	* if (dwater>0 , {1.Ca.solu	<pre>ution}, {2.Ca.solution})")</pre>			
$@Calc: (1, "1.Ca.d = \{1.Ca.$	d} - dmass")				
$@Calc: (1, "2.Ca.d = {2.Ca.})$	d} + dmass")				
@globalvar: 1.Cl.solution 0					
@globalvar: 2.Cl.solution	. 0				
@Var: 1.Cl.d 0					
@Var: 2.Cl.d 0					
@Var: dmass 0					
-					
<pre>@Calc:(1, "dmass = dwater</pre>	* if (dwater>0 , {1.Cl.solu	tion}, {2.Cl.solution})")			
$\[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \] \[\] \] \[\] \\l\)\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\$	d} - dmass")				
$\[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \] \[\] \[\] \] \[\] \] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \[\] \[\] \] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \[\] \[\] \] \[\] \] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \[\] \] \[\]\\\l\\)\\\\\\\\\\\\\\\\\\\\\\\\\\\\\$	d} + dmass")				
Aglobalvar: 1.E.solution 0	-, ,				
Aglobalvar: 2.E.solution	0				
@Var: 1.E.d 0					
@Var: 2.E.d 0					
War: dmass 0					
evar. anabb o					
@Calc:(1 "dmass = dwater	* if (dwater>0 /1 E solut	tion) (2 E solution))")			
θ Color (1 = 1 = d = (1 = d)	- dmacs()	(2.2.301001007)			
(Calc:(1 2 E d = (2 E d)))	+ dmass")				
(1, 2.5.4)					
alobalvar: 2 H colution	0				
War: 1 H d 0	Ŭ				
eval. 1.n.d o					
eval. 2.n.d 0					
eval. dmass 0					
	* * * € / ********** (1 ** -= 1)				
α	- dmacs")	(2.n.solution))")			
$\{0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 1, 0, 0, 1, 0, 0, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0,$	- dmass")				
$\{2, H, d\}$	+ umass")				
egrobalvar: 1.K.solution 0	•				
egiobalvar: 2.K.solution	0				
eVar: 1.K.d 0					
evar: 2.K.d 0					
@Var: dmass 0					
No input file or directory selected.					

Here you can see the expressions written out for all the primary entities. This demonstrates that in case of ORCHESTRA not only for the chemical part, but also for the transport systems you have access to all the equations/expression involved at the lowest level.

ORCHESTRA uses the same calculator/ solver for chemical as well as transport calculations!

So the syntax and use of objects/templates etc. is the same!

The definition of dispersion is very similar to that of advection:

🛓 ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores) — 🛛 🛛 🗡							
<u>File Run T</u> ools <u>H</u> elp	File Run Tools Help						
			1	Intro			
dispersion.inp	Read	Write	Text View	Description			
<pre>@include: parameters.txt</pre>				parameters			
				initial_solid_composition			
@Class: disperse (name, disp	ersivity, phase)			chemistry1			
This object is used to calcu	late dispersion of a solute	driven by its		chemistry2			
concentration gradient, (mat	erial) dispersivity and por	e-water velocity.		advection			
It uses the concentrations i	in both cells, the distance l	between the cells (dx)in met	er, and the water flow (li	dispersion			
J = in liters/s				concert			
D = m				feed			
				column			
Nar: 1.T 0 // flux	of water in liter/sec defin	ned in cell		outputsolution			
@Var: 1. <name>.<phase></phase></name>	0			outputprofile			
@Var: 2. <name>.<phase></phase></name>	0						
@Var: 1. <name>.d 0</name>							
@Var: 2. <name>.d 0</name>							
@Var: <name>.D <dispersi< td=""><td>vity> // m</td><td></td><td></td><td></td></dispersi<></name>	vity> // m						
@Var: 1.dx 0	<pre>// half cell thickness</pre>	(m)					
evar: 2.dx 0	// half cell thickness						
evar: dx 1	// the local dx variab.	ie with default value					
@Calc:(1, "dx = 1.dx + 2.	dx") // distance between two	o cell centres					
// Calculate concentratio	on gradient in (mol/m3)/m						
Var: <name>.dc 0</name>	$0.0 \pm (12 + n - n - 1) = (1)$						
ecare. (1, "Chame>.ue = 10	({2. <name>.<pnase>} = {1</pnase></name>	. <name>. <pnase>}) *)</pnase></name>					
//Calculate the transport	ed amount in mol/s						
@Var: <name>.J 0</name>	// delta mass for this com	ponent,					
@Calc:(1, " <name>.J=(-{<n< td=""><td>name>.D} * {<name>.dc}/dx) *</name></td><td>abs(1.J)")</td><td></td><td></td></n<></name>	name>.D} * { <name>.dc}/dx) *</name>	abs(1.J)")					
//Add transported amount	from the mass changes per t:	ime in both cells					
<pre>@Calc:(1, "1.<name>.d = {</name></pre>	1. <name>.d} - {<name>.J}")</name></name>						
<pre>@Calc:(1, "2.<name>.d = {</name></pre>	2. <name>.d} + {<name>.J}")</name></name>						
3							
Gclass: component(name)/							
@disperse(<name>, "@dispe</name>	ersivity()", diss)						
}	·····						
<pre>// This automatically includ</pre>	les dispersion for all selec	ted components					
@include: chemistry1_compone	ents.inp						
			•				
No input file or directory selected.							

In this case the amount of mass transfer is determined by concentration difference between the two connected cells, the distance between the cells, and the water flow. Note that as a result dispersion stops when the water flow is stopped (in contrast with molecular diffusion). Again you can check the expansion process by clicking Text view to see the literal calculations:

🗟 ORCHESTRA-Composer (Running on Windows 10 with 23.0.1 Oracle Corporation, using 24 processing cores) - 🗆 🗙					
<u>File Run T</u> ools <u>H</u> elp					
				Intro	
dispersion.inp	Read	Write	Expanded View	Description	
// mbig automatically includ	an dignomption for all coloct	od components		parameters	
War: 1 T 0	es dispersion for all select	ed components	-	initial_solid_composition	
eval. 1.0 0				chemistry1	
eval. 1.ca.diss 0				chemistry2	
eval. 2.ca.diss 0				advection	
eval. 1.ca.d 0				dispersion	
War: Ca D 1 1e-6				concert	
eval. ca.b 1.16 0			=	feed	
				column	
@Var: 1.dx 0				outputsolution	
War: 2 dx 0					
eVar: dx 1	1			outputpronie	
$\Re Calc: (1 dx = 1 dx + 2)$	dx")				
eouro.(1) un - 1.un (1.	un ,				
@Var: Ca.dc 0					
PCalc: (1, "Ca.dc = 1000*({2.Ca.diss} - (1.Ca.diss))")				
	(, (_, (
@Var: Ca.J 0					
$(Calc: (1, "Ca, J=(-{Ca, D}))$	(Ca.dc)/dx = abs(1.J)				
@Calc:(1, "1.Ca.d = {1.Ca	.d} - {Ca.J}")				
$@Calc:(1, "2.Ca.d = {2.Ca})$	$.d$ + {Ca, J}")				
@Var: 1.J 0					
@Var: 1.Cl.diss 0					
@Var: 2.Cl.diss 0					
@Var: 1.Cl.d 0					
@Var: 2.Cl.d 0					
@Var: Cl.D 1.1e-6					
@Var: 1.dx 0					
@Var: 2.dx 0					
@Var: dx 1					
@Calc:(1, "dx = 1.dx + 2.)	dx")				
@Var: Cl.dc 0					
@Calc:(1, "Cl.dc = 1000*({2.Cl.diss} - {1.Cl.diss})")				
@Var: Cl.J 0					
<pre>@Calc:(1, "Cl.J=(-{Cl.D})</pre>	* {Cl.dc}/dx) * abs(1.J)")				
<pre>@Calc:(1, "1.Cl.d = {1.Cl</pre>	.a) - {C1.J}")				
<pre>@Calc:(1, "2.Cl.d = {2.Cl</pre>	.a; + {CL.J}")				
evar: 1.J 0					
evar: 1.E.diss 0					
evar: 2.E.diss 0					
evar: 1.E.d U					
evar: 2.E.d U					
evar. E.D 1.10-0					
				4	
No input file or directory selected.					

In the accompanying Excel spreadsheet the ORCHESTRA output is plotted on top of the PHREEQC graph, (I will make a better graph later) and there is excellent agreement between the PHREEQC and ORCHESTRA results!



The zipped folder contains all the necessary files (PHREEQC input file, ORCHESTRA complete model and input files) to reproduce the calculations yourself.