Scientific Notebook #797

Using TOUGH REACT to Simulate Flow and It's Corresponding Interactions in 2&3-Dimensions

could reach the drupt

Specifically Looking for Corrosine Chemistics that

2	BOOK NO. PROJECT
PAGE	
location:	
Program -	Asimulation program for Non-isothermal Multiphase leachire
description	grochemical Fransport in Youriady Saturated Geologic Media.
	elt consids ig ten egention of Sale modules, However the correct Version
	is distributed with only six of them. Toushieart is a program written in
	Fortian 77 and Twons of the los prompt it pe with windows AP
	was osed
Input Files	The inset files will be created by altering Misting
	tiles in order to resemble the chemistry and borrounding
	noch units found around and above the potential drift.
	Various water chemistics will be used as initial input;
	they inclode, pore, alkaline, we what, and Ca-Cl rich waters.
	Sperifically toughteout example problem #4-(Hater-test)
	will be used and slightly modified. This existing problem is already
	charges red to be node, like allowing presipt water infiltration
	Charges seed to be nade, like allowing presipt water infiltration
	and possible changes to time step 100+put times.
	Thre is a possability that ibrehole samples that pot high on
	the aperdiagrame, indicating high Ca+Mg plus high Solfak +Cl
	Concentrations, will be used as starting pre-water Composelons.
	This initial water Chamistry, that has the potential to be corresive,
	would be runthrough the rock units that he above the
	potential drift. After the nodel predicts water-rock
	interactions, the resulting water chemistry will be
	evaporated to see y corrosive waters form.
	Liker
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Wa	actornant example	problem #4. ancorporer to see the effects, if an	China
3	Techana into maha	on to see the ellerte if an	(1)
	The state of the people	and the special state of the s	7
<u>A</u> .	Chemical inp Change th	es surrent water composition	tions to 1
3	pure water injelier pl	us rurent water composed	isn.
	Add to Gener file be	term) Source Heo Comming a	has
	train water		
	Created Juxna outo	of files flow, out and ronl	og. out
:	* frost really wissing)	nontheoriginal polder cl	urabgiven
	The user defined on	popules are beaux.	
6K	be Cooy and pasting, line	Grener files indicates in floxege in tome (From a haining class). The	water, from
	the Ote + toff fues gives	n tome (from a haining class). Th	en
	Change and & to are	tresent in current lile	
	Program 4 2012 Tipn	to abit, then freeze	ion the
	autile competted		
8)	entire compettes.		
1.			
	166	2.16	7
7	Dame the SCINSC	sinklyance your own	same!
	Change Flow to similare	y foord in fle gren to n	re by
	phandrika 1 kg/Day.	9 day = 1,57e 5 Kg/sec	*
	8	640sec	
	enthalix to in 5/ha	promintement use 7561e	5
		, N	
	Used grid cell Mo 03/	Stalls 60+ byone Cyri	s complete
	However he lile is not	to to run for 2,7540s.	
\bigvee	Tried various rates Lingston		
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4	BOOK NO. PROJECT	
PAGE ,		i
15 date	(1) \ 2 \ \ \ \ \ \ \ \ \ \ \ \ \ \	
(0 4)	6/6-made apaph of X72 Coordinates for problem #4 8)	
W 171	took graph to see what guidcells reside at the top of	
	the grid.	
	they are as Pollows one of each Fracture F and Mohia M	
	700-8 6-706	
	700, 695, 690, 684, 713,712, 657,571, 631, 632	
	603, 609, 614, 619.	
		1
_	heron problems with m 700 as beginning gold block	
	Stating that the part B blocks (total 14) woold also	
	allew the same infiltration rate across the topq	
	the Grid. Dot sure is you need to specify the Next 27	
	Blocks because each aprid block is broken	·
	into Fractive Matrix & black.	
	File fan to completion - even created a Saver File, where	
.0	it had not before.	
\$ }	-Comparefiles	· · · · · · · · · · · · · · · · · · ·
(610		
ació	to used nisinal chemical Inpiwithout changing any	
	also Changed Printown Frequences in Solote, in phle	
1	topo. The Creased error	
	TO (INC.) THE COMPANY WOOD	
	Pack to micinal print out the coency	
	Back to original print out suggercy De Changed in Gilhation to one guid Front Intool	j.
	Same Erron Message -	
	Recopied original data back into Rollin is changes	
	Recopied original data back into folder, no changes an est get seen to complete.	•
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cella	Tracture to Sorface area of Matter inorder to	
	Tracture to Sorface area of Mathix inorder to	
	Coloulate how morn infeltation should be specified	for
	the Fractures and Matry, (these #5 will eventually be	•
	divided by 14 be cause there are 14 Manix + 14 Arachive of	aid
d	beocks that wake the upper barrary	,
_		
419/	- With All other windows Closed Because previously runs	all
	faced or Froze composer) is sated injultation at the topulant cll	P.
	Do more Erros messages, However it did Not compute	
	beyond time=0	
	Changed Gener Rile back to having undelikation	
i	Changed Grener File back to having infilitation all in one call. Composer didril lock op, However du	dn'J
~	Complete Reen	
(9)		
(4).	2100	
	To figure the difference in sorface area (SA) Between	7 the
	Fractore and Mahu pride along the top of problem	A4's
:	gred black (28 intotal) in order to correctly divide	the
	import a infelhation, el nade an ince el spra	
	I wanted down the SA of the area, between	
	Grid Cold Hothe lift and to the light and the S	Α.
:	between the color in the top row with the cell	<u>۵</u> ``
1	that his below, ilt appears that the natio of	
<u> </u>	Sp between the matrix and tracker cells a	
	the Sane,	
X	48 //.	
8)	2/8/08	
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6 PAGE	BOOK NO.	PROJECT	
	6/13/10 nan the original files on	co none-roally need	
	to add Tixtual memory.		3
	Working on the SA problem, Do	age loog the tough	
	manalo m Fractives 618/00 Concles u	o Repetile surface areas	
	minuals on Fractives wills u	was Coloulated from the	
	fractice - matin interface fractice procity, and the mine	areal volume ratio, the	
	fractic procity, and the mine	ral volume fractures.	
	clartuacy took a look	at volume larea	
	The rolume cominging from the	he ELSMENT keyword in	
	the mesh file and il trie	ed it with 3 different area	
	values - the area to the if	to the gridcoll, and to	
	The right of the gridcell Car	reabetiven collos, and area	
	between aprid ale and the		
	I then added up the nation of the feachies, il then book.	for all the native then all	
and the state of t			-d
	is by the total natio- cl got	+ the same results for all	
	three area robones - 99. 349	's of the SA late belonged to the	he
	Matrix, 1016/0 belonged to	o the practores.	
		5 9921 / 1276	-(+-
	So the matrix infilhation = 1.57c - Fractore injuhation = 1.57c	"> Kalsec " 30,7 134 / 14 = 1,114e	-9
	Fraction = libte	"hallec * , oou 6/14 = 7,4012	
<u></u>			
- ^	Enter in the above date , using p	revious enthology to Update	
	the GENER file.		
·			
	2808		-
•			
			-
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the file Ran, and got forther Lin Flow rile) than it had byone. However, when I try to report run either the program Quits with a Domain Singerror or acts as it has completed, but the file hove not conto the end.

el coeculate de the injettation rate per cell incorrectly.

el used the volume of each cell to calculate the rolume fractore

volume, this was multiplied usly the Surface Area Fraction

voli Volume for each cell. SAMETO which was then Multiplied

by the unfitation rate of 157e-5 Halsec See Table

					والمراضين		Approximate the second		34		
ij	#						,		sa frac*vol		
	across	40	· -							f	
1	77		x	У	volume			sa fraction		frac*infiltration 1.08929E-08	
		f 700	-8.150E+01	8.419E+01	2.981	0.00660125	16.25			1.63923 E-06	Î.
		m 700	-8.150E+01	8.419E+01	448.600	0.99339875	16.25		0.104409		
		f 695	-6.600E+01	8.419E+01	2.522	0.00659999	13.75			9.21526 E-0	<u> </u>
		m 695	-6.600E+01	8.419E+01	379.600		13.75				
1		f 690	-5.400E+01	8.419E+01	1.903	0.00660069	10.37	0.067072	0.000443		<u> </u>
	3	m 690	-5.400E+01	8.419E+01	286.400	0.99339931	10.37	0.067072	0.066629	1.04608E-06	
	4	f 684	-4.525E+01	8.419E+01	1.490	0.00659905	8.125		0.000347	5.44461E-00	<u> </u>
	4	m 684	-4.525E+01	8.419E+01	224.300	0.99340095	8.125				
	. 5	f 713	-3.775E+01	8.419E+01	2.119	0.00660086		0.052552	0.000347	5.4461E-09	
1	5	m 713	-3.775E+01	8.419E+01	318.900	0.99339914	8.125		0.052205	1000	\vdash
-	6	f 712	-2.200E+01	8.419E+01	2.977	0.00660122	9.685	0.062641	0.000414	197	
3	6	m 712	-2.200E+01	8.419E+01	448.000	0.99339878	9.685	0.062641	0.062228	1000	
	7	f 657	-5.000E+00	8.419E+01	2.466	0.00659948	11	0.071147		7.37164E-09	_
	7	m 657	-5.000E+00	8.419E+01	371.200	0.99340052	11	0.071147	0.070677	1.10963E-0	ŀ
		f 571	5.000E+00	8.419E+01	2.466	0.00659948	11	0.071147	0.00047	7.37164E-	<u> </u>
_		m 571	5.000E+00	8.419E+01	371.200	0.99340052	11	0.071147	0.070677	1.10963E-	Ì
		f 631	2.200E+01	8.419E+01	2.977	0.00660122	9.685	0.062641	0.000414	6.49211E-	1-
		m 631	2.200E+01	8.419E+01	448.000	0.99339878	9.685	0.062641	0.062228	9.76979E-	1_
		f 632	3.775E+01	8.419E+01	2.119	0.00660086	8.125	0.052552	0.000347	5.4461E-	
		m 632	3.775E+01	8.419E+01	318.900	0.99339914	8.125	0.052552	0.052205	8.19614E-07	1 –
		f 603	4.525E+01	8.419E+01	1,490	0.00659905	8.125	0.052552	0.000347	5.44461E- 09	
		m 603	4.525E+01	8.419E+01	224.300	0.99340095	8.125	0.052552	0.052205	8.19615E-07	}-
•		f 609	5.400E+01	8.419E+01			10.37	0.067072	0.000443	6.95073E-09	1_
		m 609	5.400E+01			0.99339931	10.37	0.067072	0.066629	1.04608E-06	1
		f 614	6.600E+01			0.00659999	13.75	0.088933	0.000587	9.21526E-09	1-
		m 614	6.600E+01	8.419E+01							1
		f 619	8.150E+01								\mathbf{I}^{-}
		m 619	8.150E+01							1.63923E-0	1_
	1-1-	In A 19	1 0.100L-01	1 A.LINE, A.	1.12.003	totel	154.61			~	*
						100000		**			



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8	BOOK NO. PROJECT
PAGE	No. 1 -
نواتو	2006
<u> </u>	lack
	towate problem Hwork. also I tried to after the Gener
	Con a problem with the servi
	a jew celes to be ordeled before an error occurred.
el	a few colos so de diaced bejod an over occurred.
(dn	Copied piles and lend to my nome computer. Used
	Gener file with all 28 celes across the top indicating
	injectation, the file pan" Normally" to the same point
	the example file had - with a param of 99 instead of 929.
	181417/66
6/18	ran the lite for H colls, 2 to the truly of the
	drift and 2 below. The results of the celes that
×	allowed infilhation varied little from the ones
<i>***</i>	without.
	1.
7/*	· · · · · · · · · · · · · · · · · · ·
	26 Tran H more colls 875/545/866/341 that are
	Closer to the druft, now apparent defferences are
	noted. a also ran the untire il cello (alislas)-
	En a param of 9999 for the mox timestop. Results have
	coryct been put in spreadsheet form
~~~~\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\	
7/2	· · · · · · · · · · · · · · · · · · ·
	Transfer files For a sore tests to work computers Files in Golder D: Toughreadt/ pt-ok
7/28	Tried runging til Ambiert runs at 25 and 90 degrees
	for the 4 wasterpes County) wester pore, a cland
	allaline. Il change all proper pararameter (BBC)
ANGLIOR COLLEGE	and started the Turns, tompula property up a LS
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	BOOK NO.	PROJECT	9
	1006-		PAGE
	7/3/Continue to 7	un updaked Guartyk hally turn of comp e it was going the op. Most file Compl	ambient files,
4	had to many	ially ten of comp	soter a few
	times becaus	e it was come the	ish a
_	physical dos	op. Not file compl	eted Successfully
	15		
· · · · · · · · · · · · · · · · · · ·			
	Slostinished repring	n few prodems (Erroso	mbient files
	Successfully with	n few produms (erroso	and shot downs)
	25		
<del>-</del>	Ø Ma		
	8/106	15 00 000 110 110 00	000 11.0
1	Copie a the full	Sim myers used to ex	nd Cooled
	Thomas motors	ren in toeshread a	the copied
	10 modified His	comporter (): tough reac ahemistry to create !	Le various
<u> </u>	LE TOUR CORNERS IN	nons mentioned C7/28/a	a). However.
	because CO2-21)	nit a promory species,	it couldn't be
	added to the	initial fomposition	whit hadbo
)	be geralculat	ed on HCO3 ford addd	to the existing
	concentration	of that species. A few	ominor changes
	to the chemical	Tiles and the Time	25 LDONG.
-	completed and	Ready for Comparis	<u>M </u>
·		00	-10
	15.5/2/010		
	82100		7/
			106
1			
		naday	
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10 PAGE	BOOK NO. PROJECT
	8/2/00
	Sorted date into spreadsheet form for the oxidy run obtaine
	LS .
	8/3/00
	and Satisation (Ligard) Changes. Altered Flow and Soloke Ches to reflect the cells is want to look at the temperature
	files reflect not moch change.
	8/7/06
	Used a Column Closes to the drift, changed only the cells to
	used a Column Closes to the drift, changed only the cells to report in the output files towerer for some romson cl heep certain an error newsage "M6202: Math"
	25 8/8/06
	for the cales clam interested in hoping that there
	was a Lyping error. However, this is not the case and the
	Re runler out expot much help classe ecropied the
	Corrupt a el neran the problem ofes on Myers Computer. Waked
	8/9/06
	classo ran the two columns of interest on 5mm
	Paran beyond to 9999. Both files Condeted with
	out prodems, However, there really is very 1, He temp
	Yariance, (2426)
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an change fourtime parameters as a fine + Erron However Each

peu hours. Checked the plantal again, wolock

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**PAGE** slem 3 ran to Completion, but the ged the profiber Eirst writing control tariable he Solite file and the Mayor from 99 to 599 cont as for a changed 9/14/010 The reen looked to complete without error opening the times dat and and asobs files its apparent the the ron Not complete to the desired time. I switched home of the aptions in the solute inp, to Allow the program to ice the prenting in order to decrease the filesizes 9/15/06 the print parameter to Coo, ther reran , I hansper copies of the files to MY Trees to see how for it could

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213/04

il ran another lot of tests and decided that il count blay in the 150°s range and under 20 hrs. chassome that the actual bench top test will require a higher heat than predicted. So clande 565/8 and side heater temp of 40. This gave 150° in 17 hours with a maxtemps 168. If a max temperature of 170-180 are acceptable the Two may complete in 13-16 hrs.

Step 3Ly Sg=1 ORC =51/day=/,93e⁻⁵ Kg/m²s over 3 cells

Lin the middle of the earge. Changed Metra TopBC (cell2426)

Started with 565/s and 40° Side heaters.

This completed in 23 min and gave an estimate that it

would reach up to 168 degrees as a high and loke it

to 150 within 17 hours. I'm hying other combinations

been if the process can be speed up.

2467 Results From part 3

Part 3 - Add .5L Heat load needed to reach 150 center in shortest time. Using Center and side heaters start Sat gas Heat Load side Temp center T-high Time yrs Hours run time Min

0.02 stopped
0.02 stopped
0.02 stopped
11.11 30
15.86 26 min
17.08 25 min
16.93 23
18.64 23

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H Next Day

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18	BOOK NO.	PROJECT		
PAGE	14107	Moved to Nakloook 863	SE 3/22/07 SS	
	Paray		•	4-
	1 by same	as pare 3, but infilhation will	be Stopped	4-
	incrious	s times (1,5,10 days to book for	funger flow.	-
	1 Times	changed (target times) we	provad sheet that	<b>-</b>
	Komes i	unded from with this books	sol. For Some	4-
	reason h	exp getting error messa	ge about recorrect	4
	data.	Note: May Home was beliebed	1 based m	4-
	<b>\</b>	4 State time from part 3 62		1_
	Lessoni	Jayos was chosen for the per	H074-	
	8	-\ @		
		×2201		
2	115/04			
	Mehal	ile fund and running.	Added a	
	line to the	2 top BC to speaky OBC	tecreased to	
	( ax sociuia	times. After each time o	step a benico	
	a anaphs in	In by made with tecplot t	o show the	
	ellects in cu	thing of the inhibitation for	achor the 16	
	time Steps a	graph of Temperature, press	ore Cignid Saturation	
	and no lastre	humidity. These will be used	to proceed to	1
	the pext to	ue estoro por injulhation, M	re Dointbeing in	
	tabitione when	. can univing effects a u	bater be seen and	
	alter how to	nci		
	38			
	<i>U</i> <b>J</b>		\	1
	2/16/07			
	Sofar il ha	eve run the same ble Dtopp	sind infilhation	
		s, and 25 hours bot much	01	1
		ere re ron with the incil	haton	1
	a plana at	3 2 14, 30, and 200 days,	mara si cai h	1
	Nag I Still Mar A	sign didn't change His	14/4/	1
	enough In II.	a Dift to show any Fincer	inc was K	1
	The N.V1111	e two with the whole a	t Disch	1
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## PAGE Mored to Note book 863E 3/22/048 tops 4 enfilhation was sed 10415, Soa ustra results of unfitation intersecting H clear. The file was run w/a cotogs of Byer and logs 15 target tomas. With the The time steps wil be adjusted accordingly he drift also by zours higher Saturahmi him of 14-1351507. carfully. Her changing larger times mento crose to land before and offer ( before and offer 104 5 year cutogo was rurun with hours target times, the yearts were the sance. 2/20/07

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er i samuello.				<b>∠⊥</b> PAGE
		Mored to pook boo	L 863t 3/22/078	
	7011616	The state of the s		
	- 20 4rs L3 2/21	107 LS	<b>1</b> • • • • • • • • • • • • • • • • • • •	
	10 yrs cuto	by 20 high sat below	buff by 30 dried a	<u>t</u>
	3 grs cuto	6) by 20 high sat labor	SSZZIZITAS back to look	at lyr
		Shows Sat Abore drift		
)	ayrs at	1.24rs 56 9 in Albation V	caches Drift, 24rs 15c	Above drift
		100yrs no infiltre		
	For 3,5	and lours cutago by 100	Durs you see Sigo ba	ck to
	Hirin	al state, 24r cutogo	does not. Dry out	only
		below Grass Lectro		
		section (2014)-		
	128			
		-89	di partini	
	2/22/07	5-20		
	_	Episodia		`
	12 ×	nuch like Part 4-9	Startdry. cut ont	In Pad tration
			11.5	
	First try	2 times/-cutor	and then pick up	
	ar hitra	Han - Yelond for spr	eadsheet the resc	o Its
•	and cr	\		
1 PREACHES	l .	Cher certain Amount form people	val Saturation	
	# 2 2,104rs V		" Bigger time	aap Hedd
	LS			
	,	,		
	2/26/07		\	5.1
	For punt 5	the cap by extra	and continued intelli	ation
	wareased	9 • • • • •		
	#3.2,30yr			
	L'orientle cana	of plates in tespertage to	o Error with CSE Alex	
	25	·		· .
	continued on	1291.23		
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22	BOOK NO.	PROJECT	
PAGE			
<i>_</i>	21/02	4 4	
2/4	la Problem H Hough near	t-continued	
2-2-	7		-
	Starting over 11 bumped	up the target time to	
-	10 yrs, the file was take		
	so a controlled C and began	n to blowly decrease	
	the file target time . after	Several runs el began	
	to increase the target time	from 2.75 yrs, even then	
	having problems with the	ili progressing	
	13		
	122104	×	
7.2101 .	75/04		
	Looking at the files some	152-22-07 tolerences May Need	
	to be aftered along with &	ome time stoos. Once the	
	he gets to 2.75 years (2.79), 7	he problem withoustenand	
	Kcyc begin.		
	15		
	2/23/04		
	Chanced Param line	2 (length time step to regati	ve)
	with no lick. Also chow	ace the maximum time Stop	
	Observe which appeared to	be too high. This caused an	
	error, I believe the book	k and file (Both Manuald do No	ł
	exactly correlate.	,	
	15		
		· · · · · · · · · · · · · · · · · · ·	
	LS,		
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Date Generated:	10/01/2006	
Operating System: (including version number)	Windows	
Application Used: (including version number)	TOUGHREACT ver 3.1	
Media Type: (CDs, 3 1/2, 5 1/4 disks, etc.)	1 CD	
File Types: (.exe, .bat, .zip, etc.)	xls, txt, eye, up, out, dat, zip, rels, polf	
Remarks: (computer runs, etc.)	Media contains: Input/output files for Hydrus	