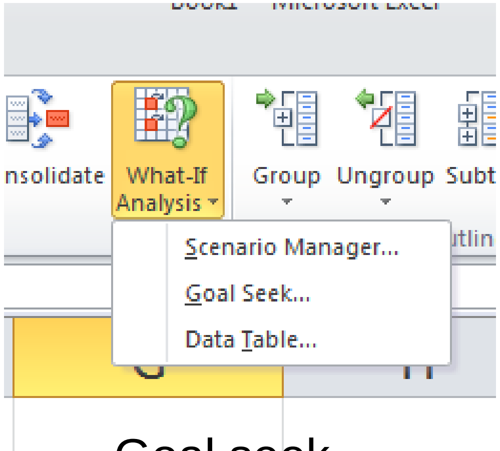
One phase flow in porous media

January-2015

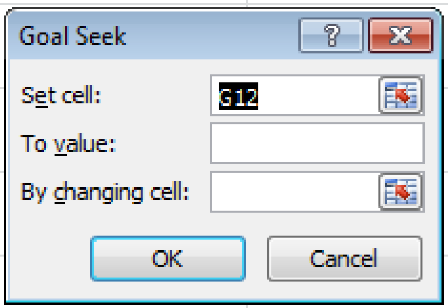
Hans Bruining

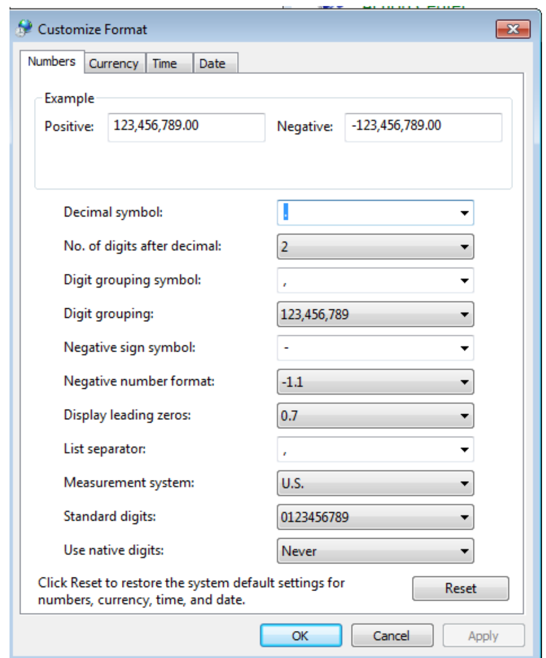
formulas

EXCEL settings

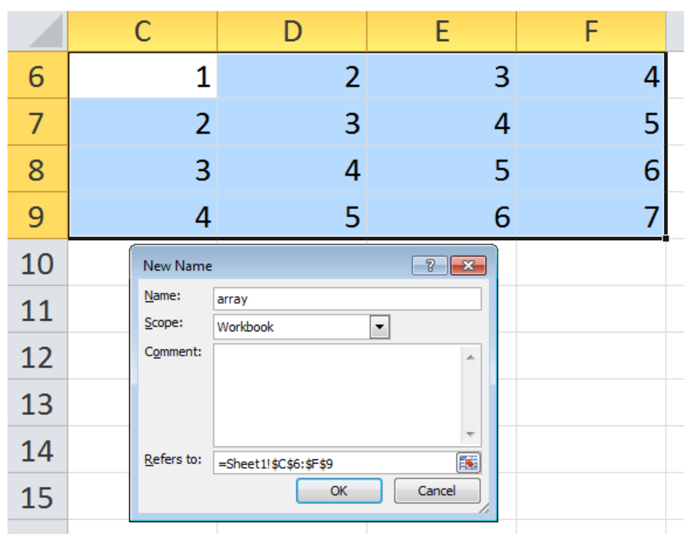


Goal seek





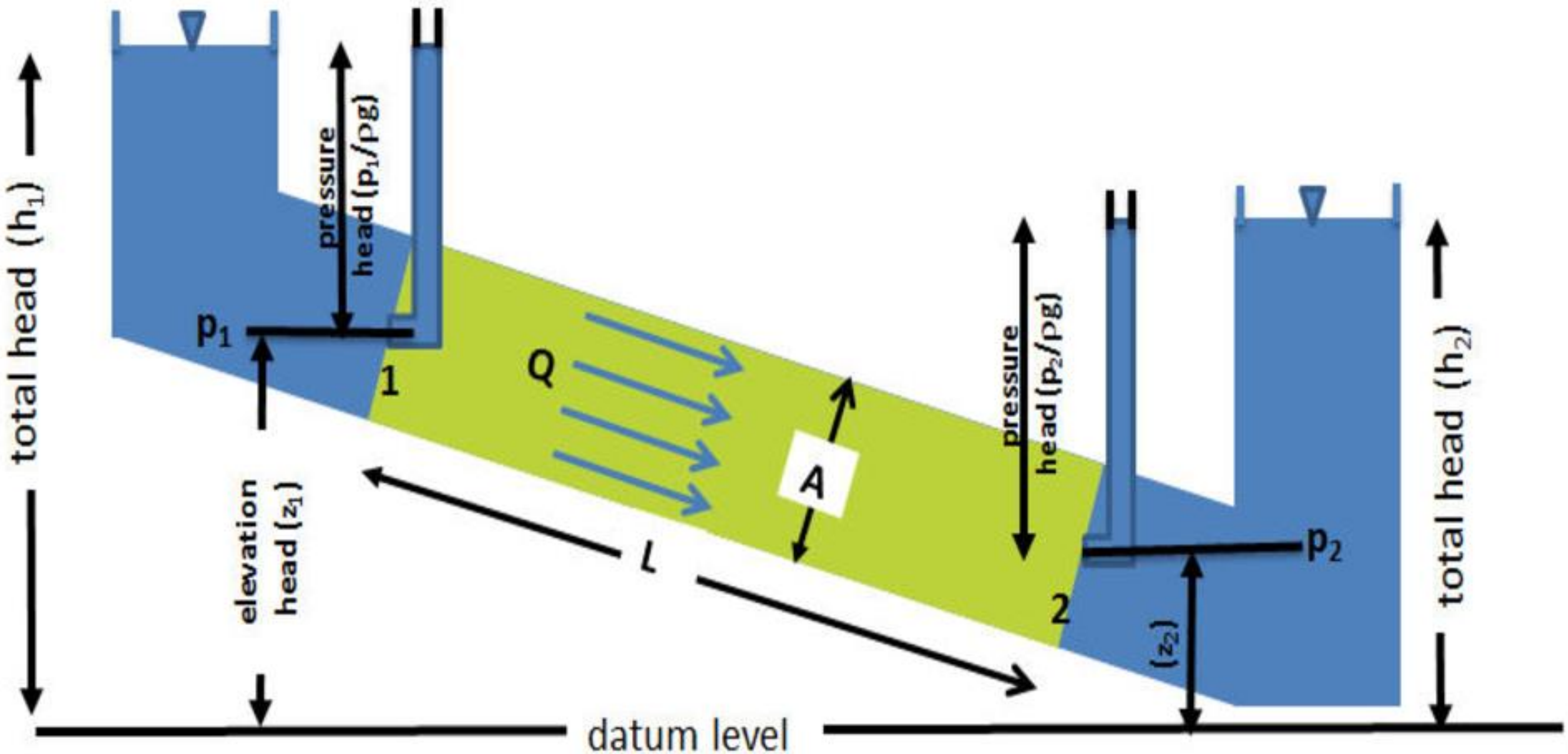
Control panel →
Region and language
→
Additional settings →
Numbers tab →
Digit group symbol



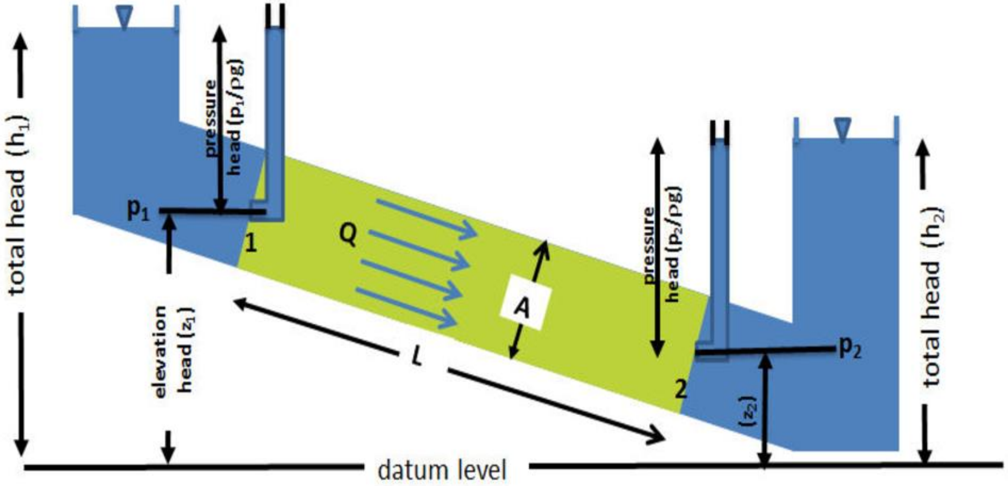
Formulas →
Define name →

=average(array)

Darcy experiment



Darcy experiment



$$Q = KA\frac{h_1 - h_2}{L} = KA\frac{(p_1/(\rho g) + z_1) - (p_2/(\rho g) + z_2)}{L}, \qquad (1)$$

where p is the pressure, ρ the density of the fluid and g the acceleration due to gravity. or in differential form

$$Q = -KA\frac{\mathrm{d}h}{\mathrm{d}l} = -KA\frac{\mathrm{d}(p/(\rho g) + z)}{\mathrm{d}l}\ . \qquad (2)$$

Nomenclature in hydrology or petroleum engineering, K = k ρ g /μ

h	piezometric head (total head)	$[m]$	$\Leftrightarrow$	Φ	potential	$[Pa]$
$\frac{h_2-h_1}{L}$	hydraulic gradient	$[-]$	$\Leftrightarrow$	$\frac{\Phi_2-\Phi_1}{L}$	potential gradient	$[Pa/m]$
$p/(\rho g)$	pressure head	$[m]$	$\Leftrightarrow$	p	pressure	$[Pa]$
$v^2/(2g)$	velocity head	$[m]$	$\Leftrightarrow$	$\frac{1}{2}\rho v^2$	kinetic energy	$[J/m^3]$
z	elevation head	$[m]$	$\Leftrightarrow$	$\rho g z$	potential energy	$[J/m^3]$
Q	total discharge	$[m^3/s]$	$\Leftrightarrow$	Q	flow rate	$[m^3/s]$
$q = Q/A$	specific discharge	$[m^3/m^2/s]$	$\Leftrightarrow$	$u = Q/A$	Darcy velocity	$[m^3/m^2/s]$
$v = q/n$	pore velocity	$[m/s]$	$\Leftrightarrow$	$v = u/\varphi$	pore velocity	$[m/s]$
n	porosity	$[-]$	$\Leftrightarrow$	φ	porosity	$[-]$

$$q = \frac{-K}{\rho g}\frac{\mathrm{d}(p+\rho g z)}{\mathrm{d}l} \; . \tag{3}$$

$$u = \frac{-k}{\mu}\frac{\mathrm{d}(p+\rho g z)}{\mathrm{d}l} \; , \tag{4}$$

Typical values

Table II, Typical values of Hydraulic conductivity or permeabilities		
Type	Hydraulic conductivity [m / s]	permeability [*Darcy*]
Gravel	3×10^{-4} - 3×10^{-2}	30 - 3000 *Darcy*
Coarse sand	9×10^{-4} - 6×10^{-3}	90 - 600 *Darcy*
Medium sand	9×10^{-7} - 5×10^{-4}	90 mD - 50 *Darcy*
Fine sand	2×10^{-7} - 3×10^{-4}	20 mD - 30 *Darcy*
Clay	1×10^{-11} - 4.7×10^{-9}	1 μ Darcy - 0.47 mD
Sandstone	3×10^{-10} - 6×10^{-6}	30 μ Darcy - 600 mD
shale	1×10^{-13} - 2×10^{-9}	10 nD - 0.2 mD

When can we write $u = -k / \mu \, \mathbf{grad} \, \phi$?

- $\phi = p + \rho g z$; Density constant
- No inertia; $-\rho \, \mathbf{grad} \, \phi = \mu \rho u / k + \beta (\rho u)^2$
- No anisotropy: $u = -(\mathbf{k} / \mu) \bullet \mathbf{grad} \, \phi$
- Representative elementary volume can be defined
- No slip

Exercise: $u = k \rho g / \mu$

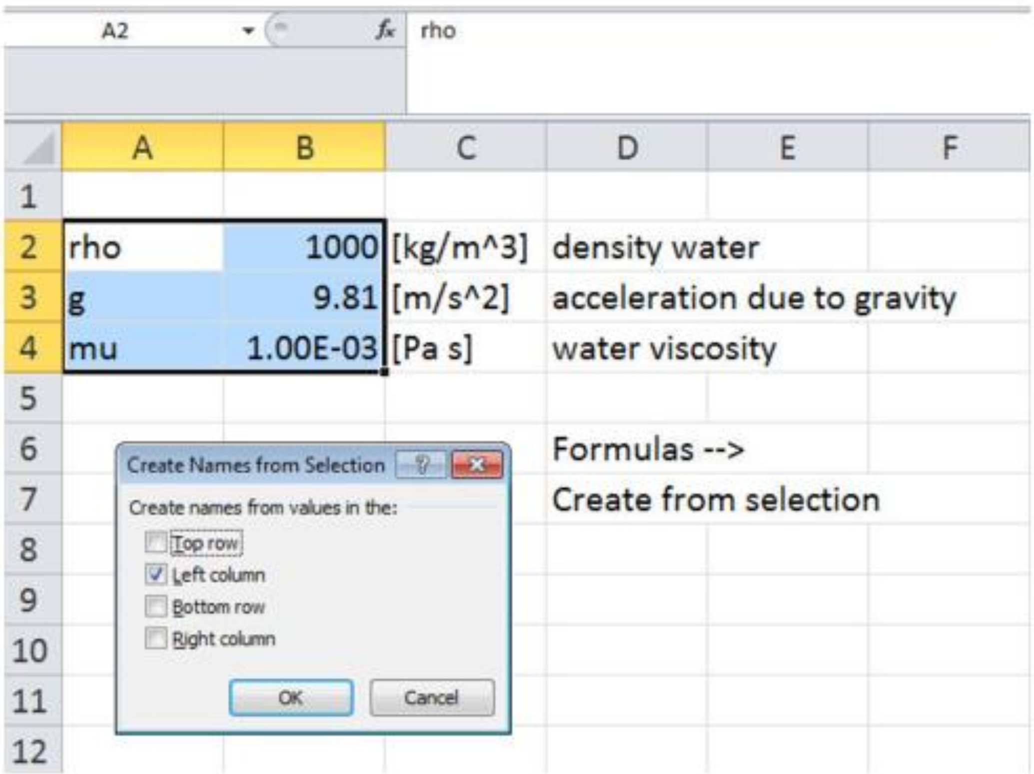
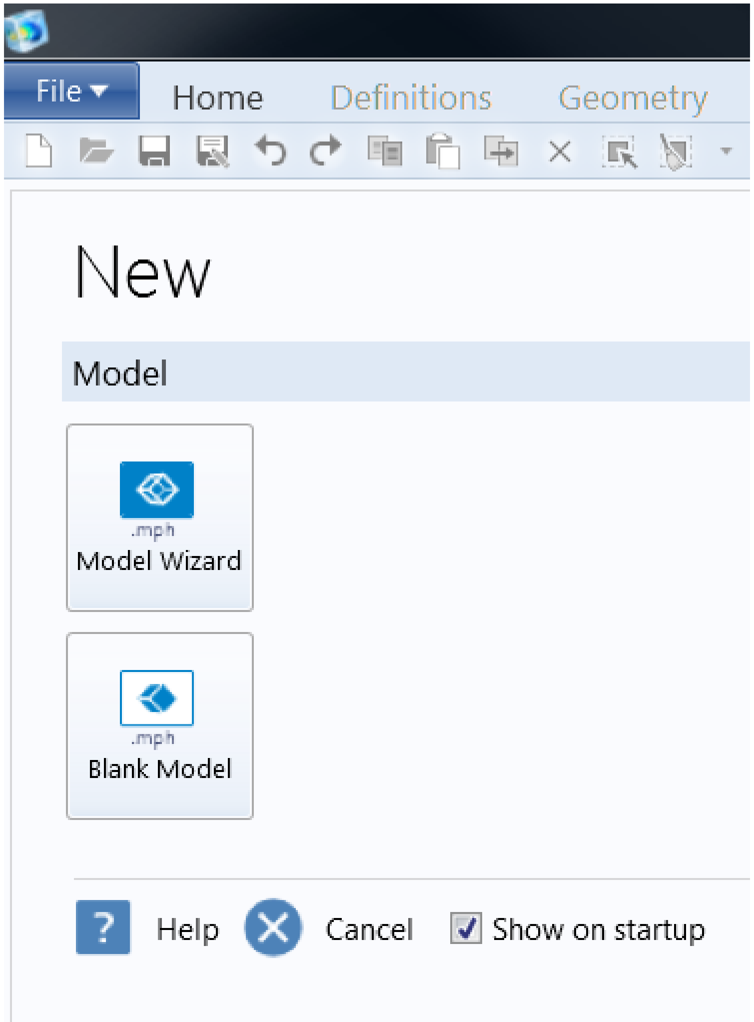
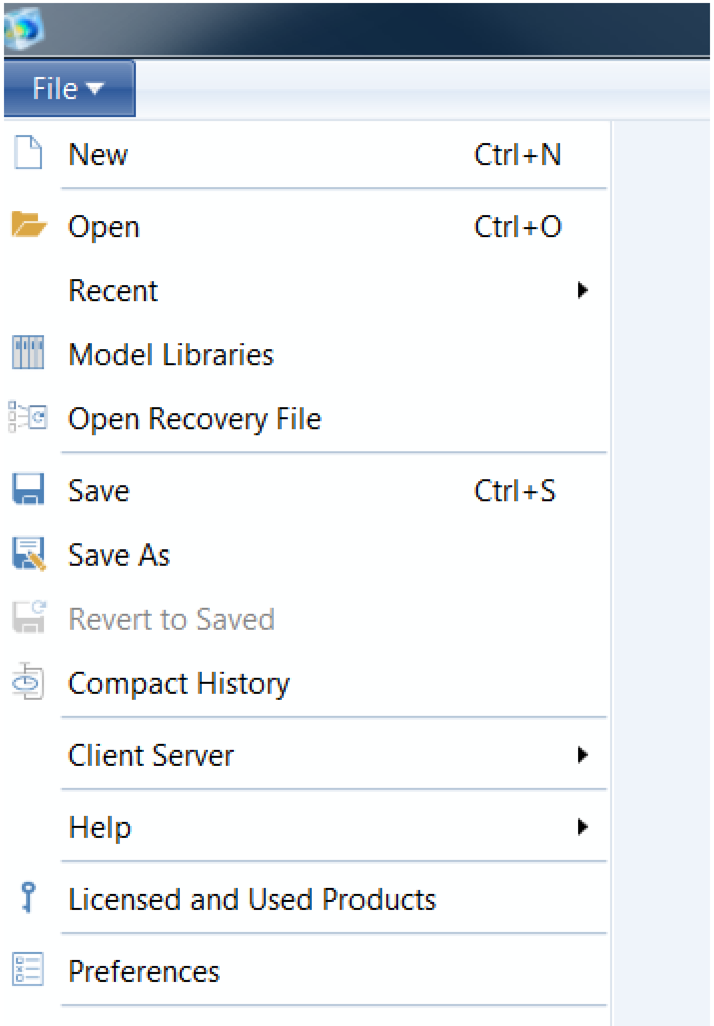


Figure 2: First highlight the cells containing the values at the right and the names at the left. In the formulas tab choose "create from selection". After clicking "OK" the cell B2 is named rho, B3 is named g and B3 is named mu.

Start-up COMSOL; press Blank Model; save as “ab.mph”





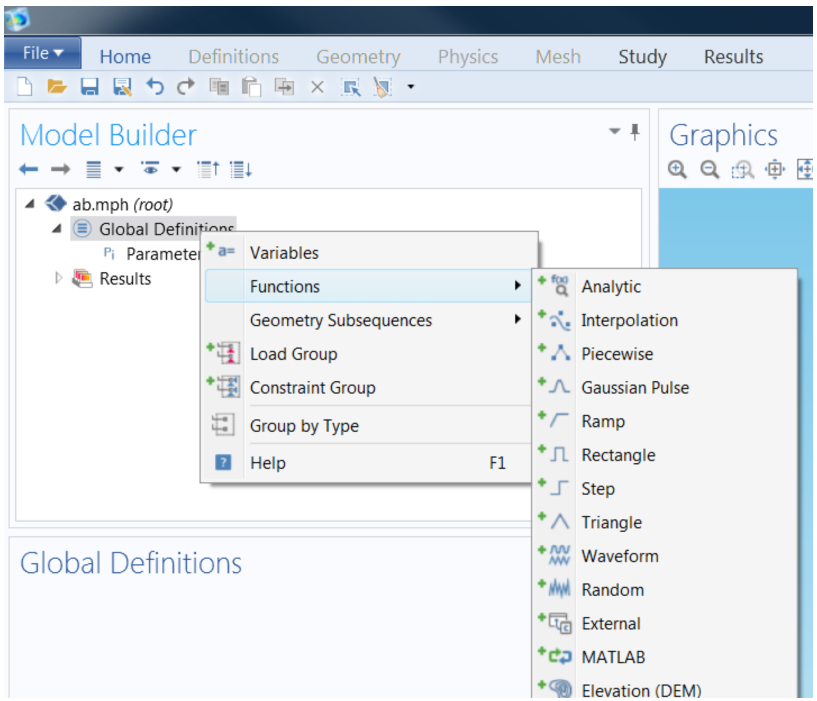
Right click parameters and parameters in COMSOL

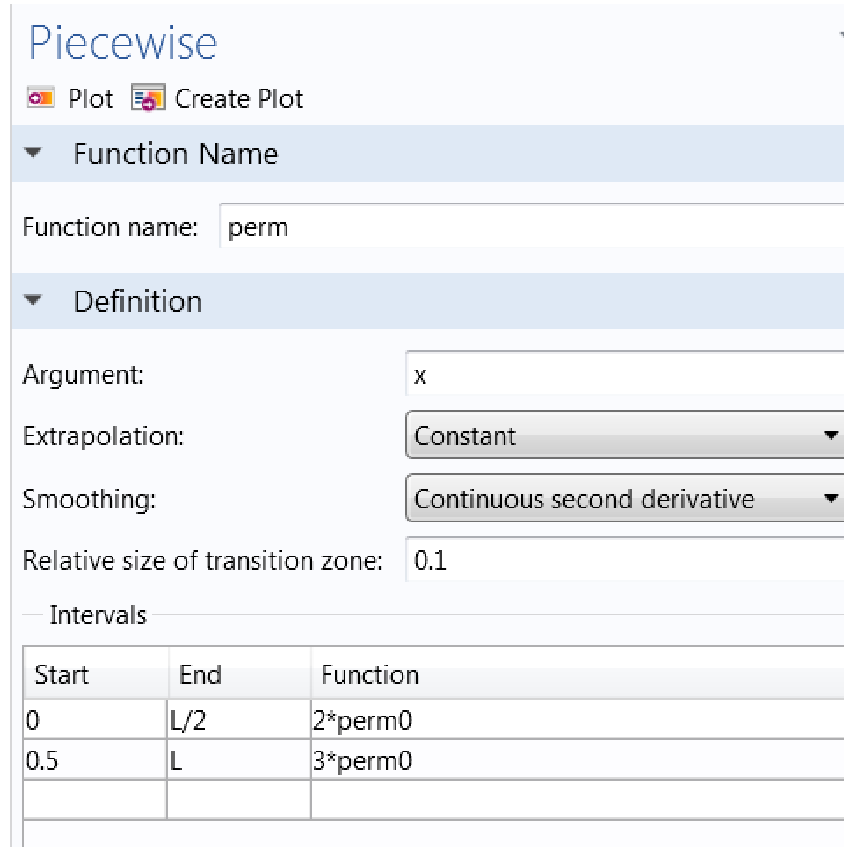
Parameters

Parameters

Name	Expression	Value	Description
rhow	1000[kg/m^3]	1000.0 kg/m^3	water density
Lw	0.5[m]	0.50000 m	water layer on top
g	9.81[m/s^2]	9.8100 m/s^2	acceleration due to gravity
L	1[m]	1.0000 m	length of sand [ack
muw	1.0e-3[Pa *s]	0.0010000 Pa·s	water viscosity
perm0	1.0e-12	1.0000E-12	reference permeability

Right click Global definitions and put a Piecewise function in COMSOL; Plot





Put in function II

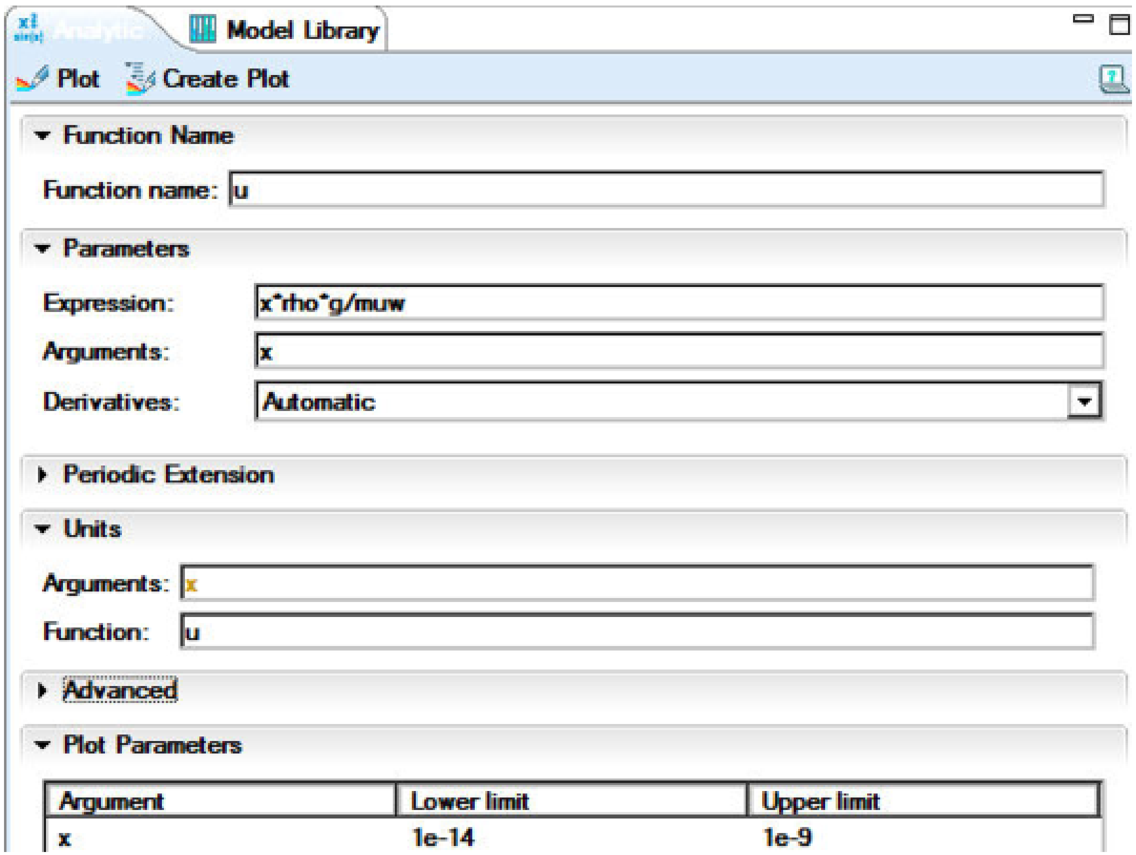
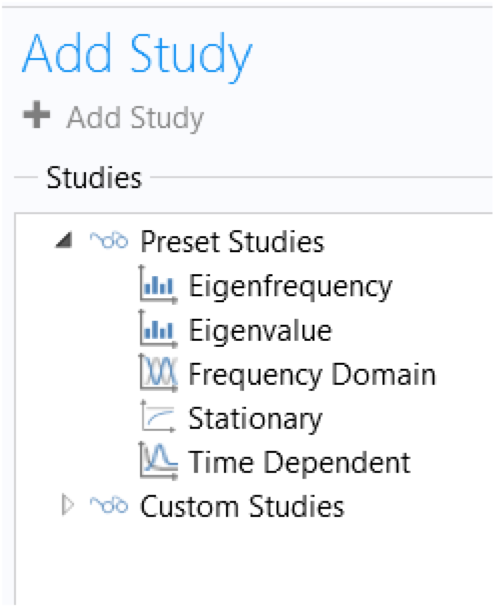
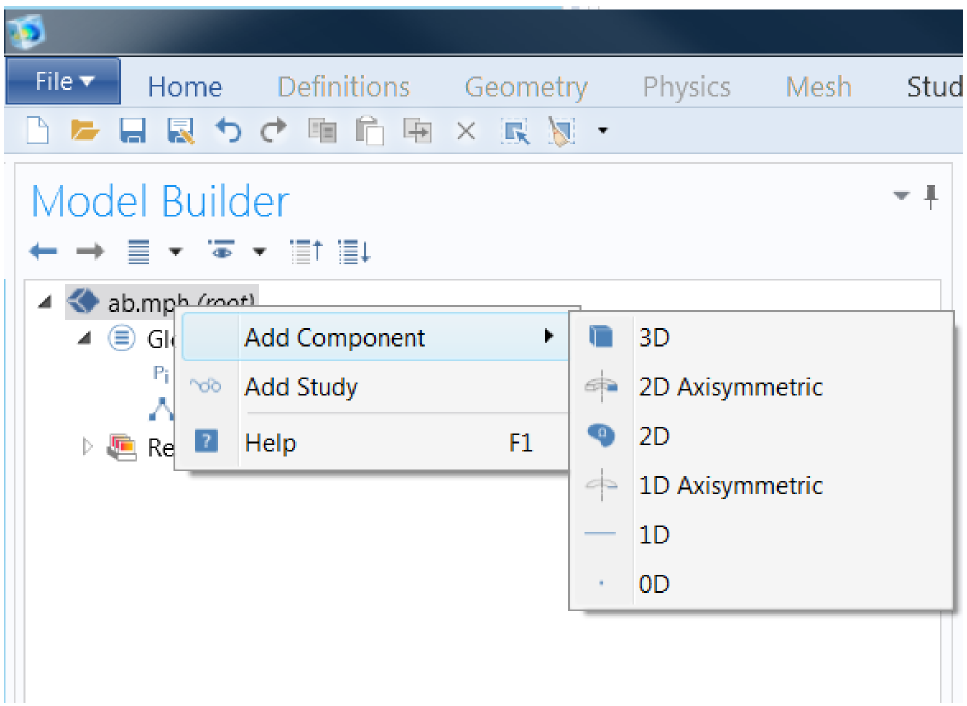


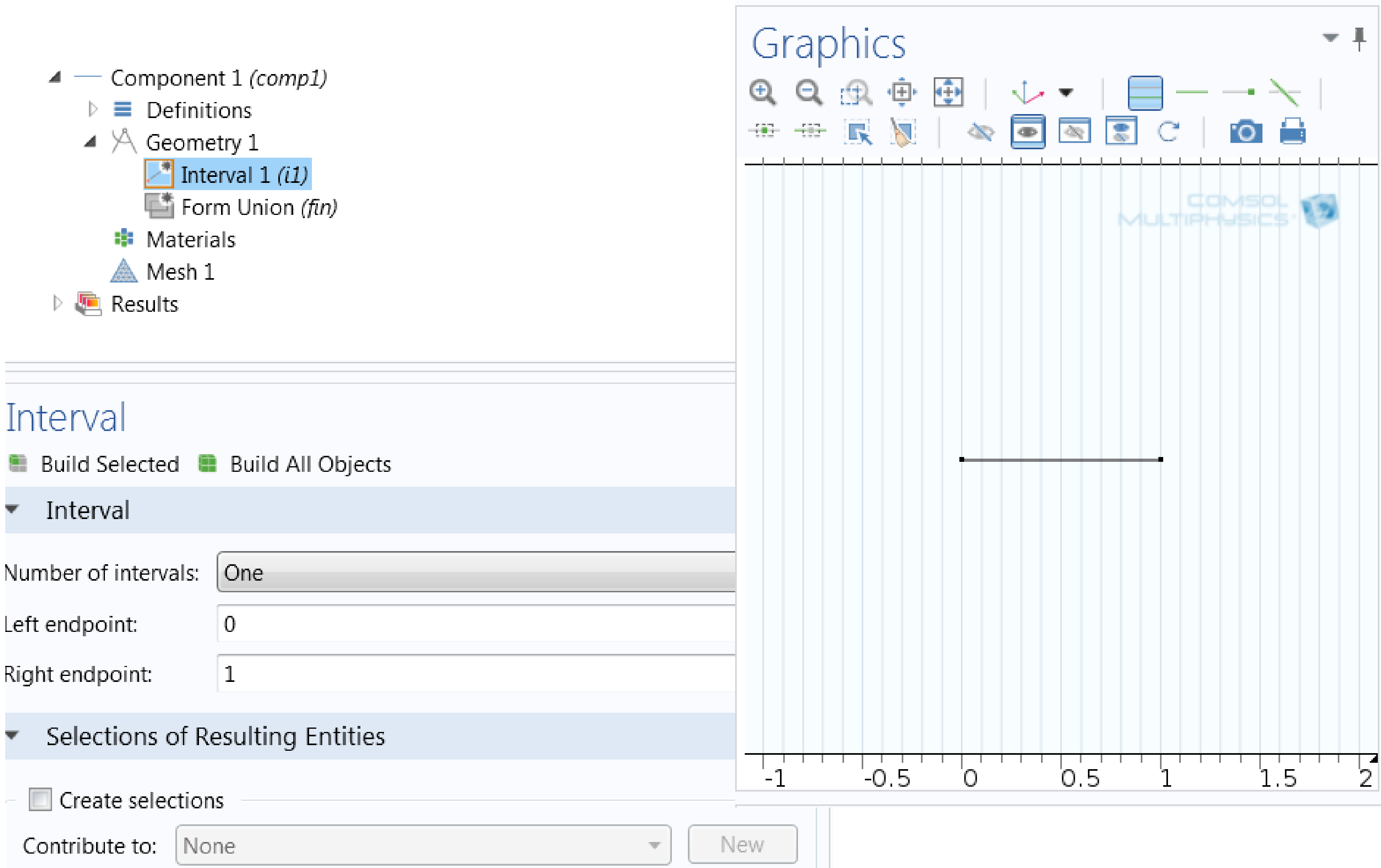
Figure 5: Right click functions → analytic. Then you get the menu shown. We use "u" as the function name. We use "x" to denote the permeability. You need to specify over what range you want to have the plot in plot parameters. Above function name press "plot". Now the plot of the function will be displayed. Above the plot, both press x-axis log scale and y-axis log scale. Press snapshot, if you like to upgrade the plots for publication. It is not the best upgrading software in the world.

Right click “ab.mph” →Add Study→ Stationary → Add component → 1-D

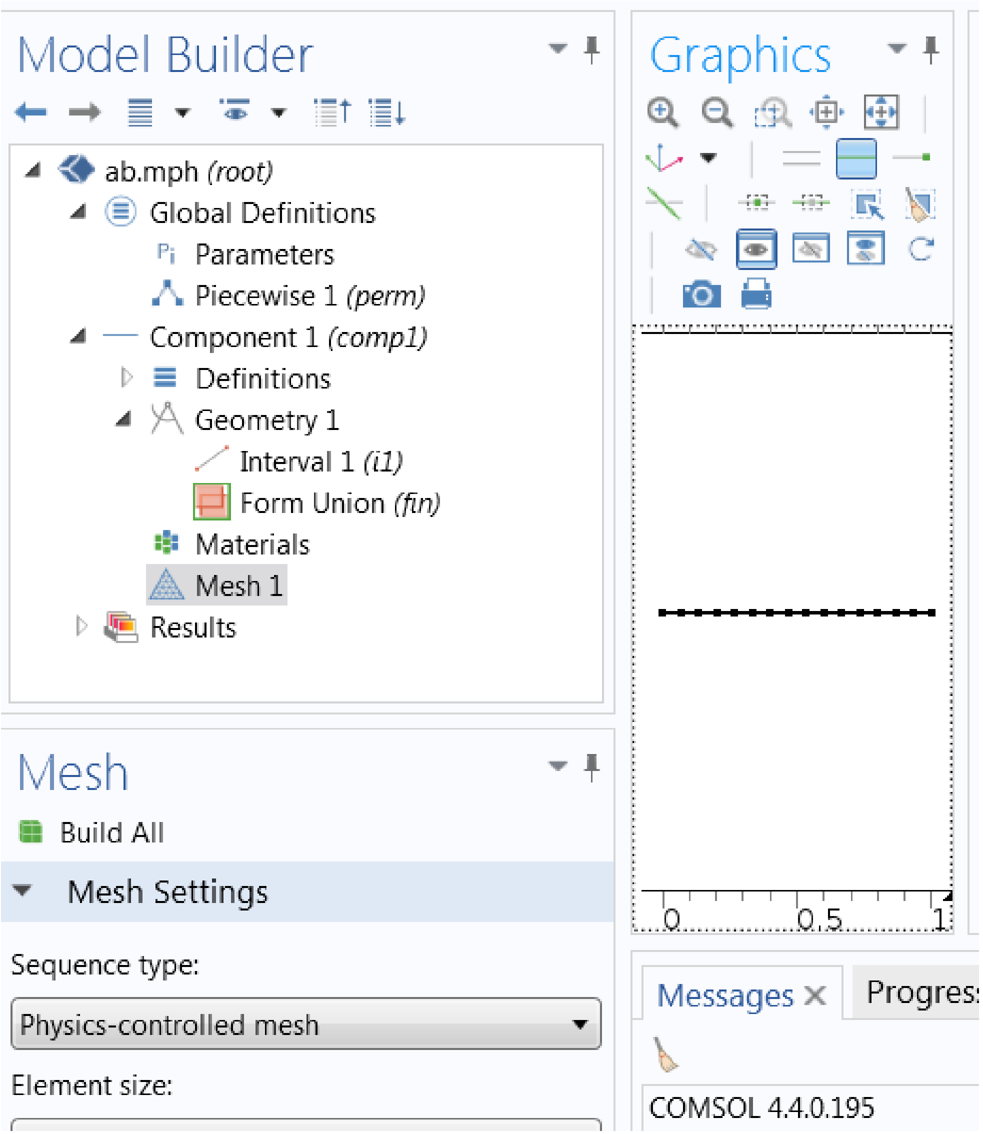




Right click "Geometry" →Choose Interval 1 → Build All objects



Left click "Mesh" → Build All



Representative Elementary Volume

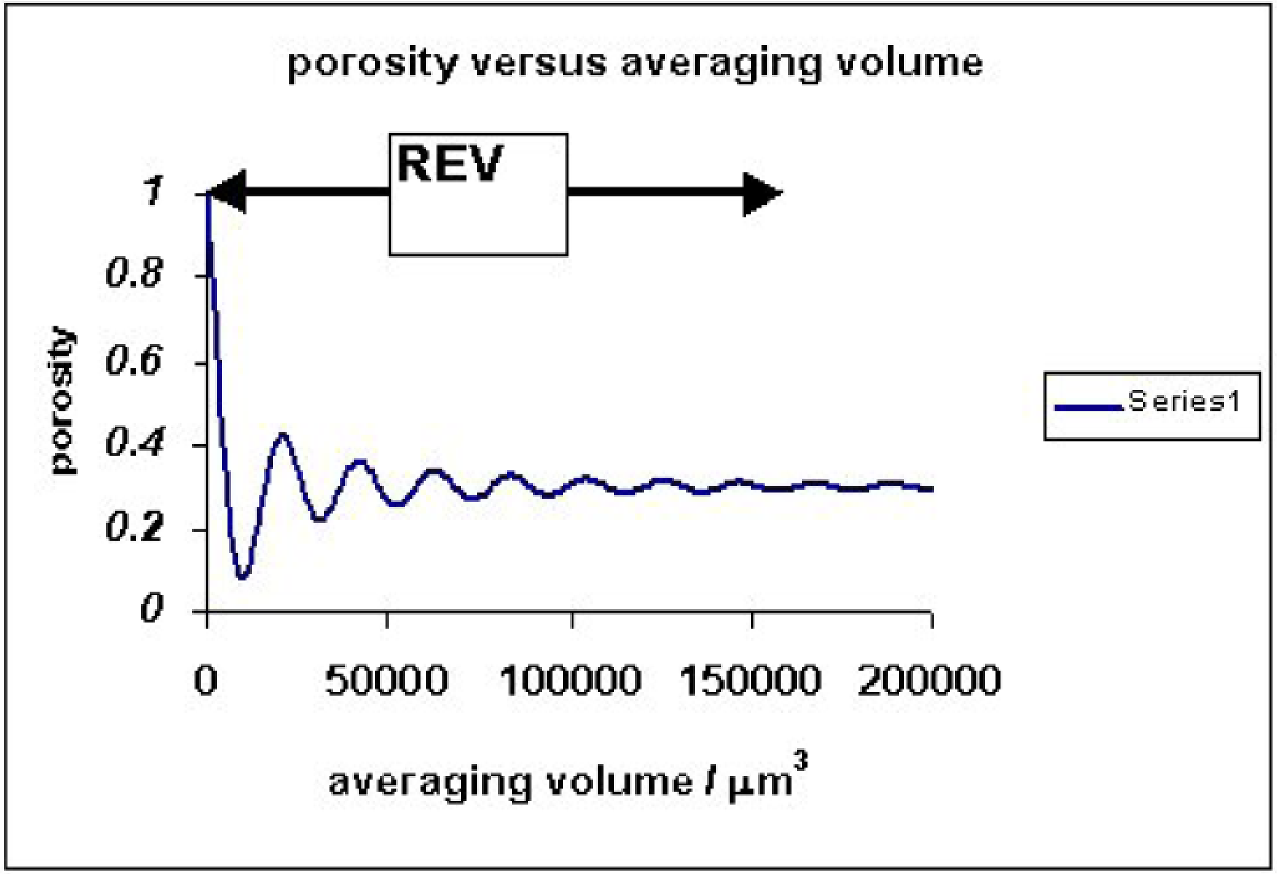


Figure 3: Definition of representative elementary volume

REV not always easy to define

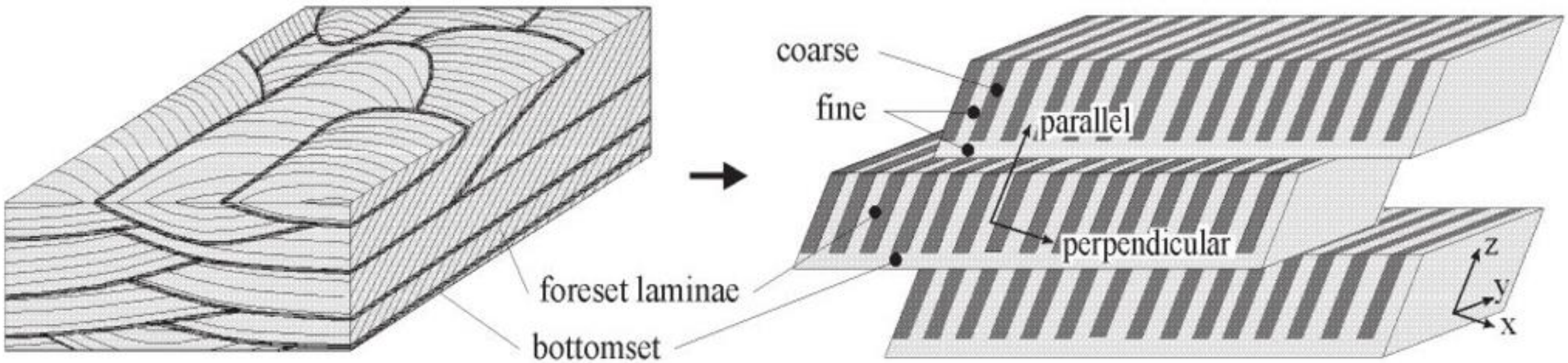


Figure 7: On the right a 3D representation of vertically stacked through cross-beds with distinctive foreset and bottomset facies. On the left the schematized model. The cross-bed sets are characterized by box like structures with a specific length, height and width. The foreset and bottom set laminae with this box-like structure have characteristic dimensions

Connection to Navier-Stokes

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = -\oint_S pdA - mg + F_{visc} \tag{6}$$

where the pressure p is directed in the outward normal direction with respect to the surface A. Note that we assume that z is pointing in the upward direction. We apply

$$\oint_S \mathrm{p}\mathrm{d}\mathbf{A} = \int_V \mathbf{grad}\ \mathrm{p}\ \mathrm{dV}\ . \tag{7}$$

This can be easily validated in cubic geometry by substitution of $dV = dxdydz$ with $\mathbf{grad}\ p = \mathbf{e_x}\partial p/\partial x + \mathbf{e_y}\partial p/\partial y + \mathbf{e_z}\partial p/\partial z$ and integration of the terms in Eq. (3) versus x, y, z respectively. When we write the mass as a volume integral over the density ρ we obtain

$$\int_V \rho\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}dV = -\int_V \mathbf{grad}\ pdV - \int_V \rho g dV - \int_V \frac{\mu\mathbf{u}}{k}dV\ , \tag{8}$$

Space dependent density

$$
\begin{aligned}
u_x &= -\frac{k}{\mu}\frac{\partial p}{\partial x} \\
u_y &= -\frac{k}{\mu}\frac{\partial p}{\partial y} \\
u_z &= -\frac{k}{\mu}(\frac{\partial p}{\partial z} + \rho g) \; . \qquad (5)
\end{aligned}
$$

The petroleum Engineering Eq. (5) is the only correct equation for non-constant densities. Typical values for the hydraulic conductivity are shown in the table

Condition density is constant

$$u = -\frac{k}{\mu}(\mathbf{grad}\ p + \rho g e_z)\ , \tag{9}$$

where we have defined the positive z direction in the opposite direction as the direction of the acceleration due to gravity; therefore the change in sign! If ρ is constant then this equation is equivalent to

$$u = -\frac{k}{\mu}(\mathbf{grad}\ \phi)\ , \tag{10}$$

where $\phi = p + \rho g z$ is the potential. Hydrologists like to write:

$$u = -\frac{k\rho g}{\mu}(\mathbf{grad}\frac{P}{\rho g} + e_z) = -K\ \ \mathbf{grad}\ h \tag{11}$$

Forchheimer equation

Forchheimer's law is an extension of Darcy's law as it takes into account the inertia term. The Equation is stated empirically and reads approximately

$$\mathbf{grad}(\mathrm{p} + \rho \mathrm{gz}) = -\left(\frac{\mu\mathbf{u}}{k} + \beta\rho\mathbf{u}|\mathbf{u}|\right) \qquad (12)$$

where we introduce the so-called inertia factor $\beta[\mathrm{m}^{-1}]$. This is all there is to know, but we gain some insight if we try to use the same procedure as above, but now including the inertia term.

Experimental data inertia

Test 1		Test 2		Test 3		Test 4		Test 5	
v	pres grad	v	pres grad	v	pres grad	v	pres grad	v	pres grad
(cm/s)	(kPa /cm)	(cm/s)	(kPa /cm)	(cm/s)	(kPa /cm)	(cm/s)	(kPa /cm)	(cm/s)	(kPa /cm)
0.547	2.779	0.44	2.779	0.429	2.367	2.51	0.1	2.51	0.512
0.972	8.027	0.972	9.1592	1.248	14.922	5.28	0.2	5.11	1.15
1.37	16.054	1.3	16.466	1.458	18.936	15.14	1.1	10.14	1.59
2.517	50.015	1.694	27.186	1.716	29.433	27.23	1.2	33.12	3.89
4.719	118.555	1.869	33.1378	3.064	81.918	32.11	1.4	44.28	5.49
4.938	182.67	1.97	38.489	4.496	172.996	53.87	2.5	58.91	8.85
4.96	129.667	2.399	65.246	4.522	165.586	69.28	4	66.37	11.52
		2.78	75.332	4.575	90.357	81.53	5.6	81.26	15.41
		4.421	173.922			94.59	6.8	95.34	17.23
		4.925	189.668			106.29	8.3	103.58	21.81

Insert trendline

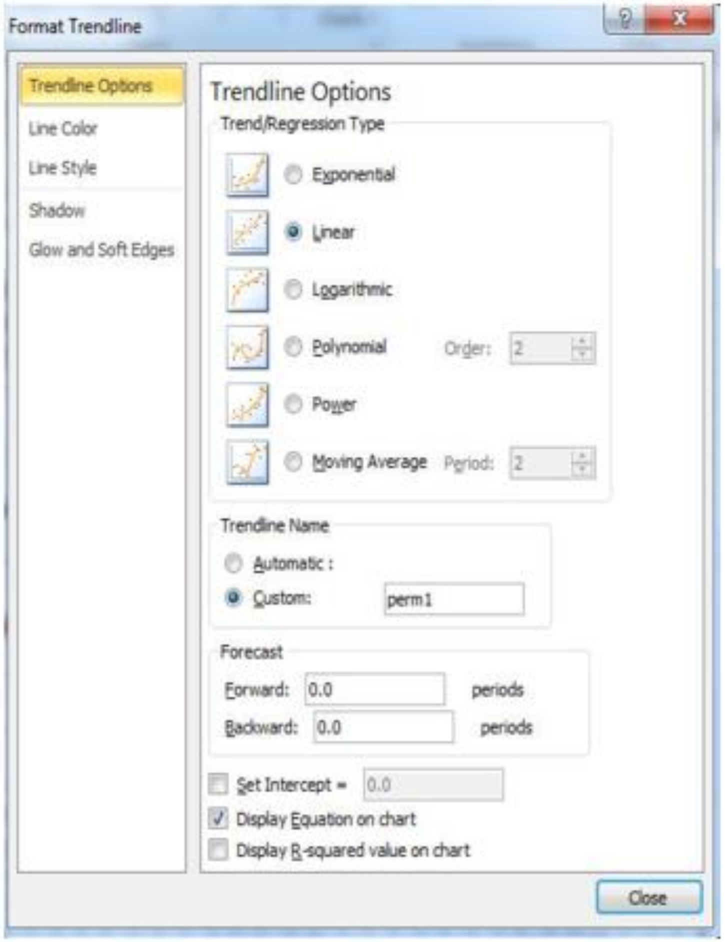


Figure 8: Right clicking on the plotted line allows to insert a trendline. Use the options as displayed

Carman-Kozeny/ Burke Plummer

$$\frac{\phi_o - \phi_L}{L} = \frac{(1-\varphi)^2}{\varphi^3}\frac{150\mu u}{D_p^2} + \frac{1.75\rho u^2}{D_p}\frac{1-\varphi}{\varphi^3} \tag{28}$$

The first term on the RHS of Eq. (28) is the Blake-Kozeny (Carman-Kozeny) part and the second term is the Burke Plummer part. It shows for which Reynolds number inertia terms becomes important

$$\begin{aligned}\frac{\phi_o - \phi_L}{L} &= \frac{(1-\varphi)^2}{\varphi^3}\frac{150\mu u}{D_p^2}\left(1 + \frac{1.75}{150}\frac{\rho u D_p}{\mu}(1-\varphi)\right) \\ &:= \frac{(1-\varphi)^2}{\varphi^3}\frac{150\mu u}{D_p^2}\left(1 + \frac{1.75}{150}Re(1-\varphi)\right) \end{aligned} \tag{29}$$

Hence at Re $=10$ the inertia correction to the Darcy flow starts to become significant.

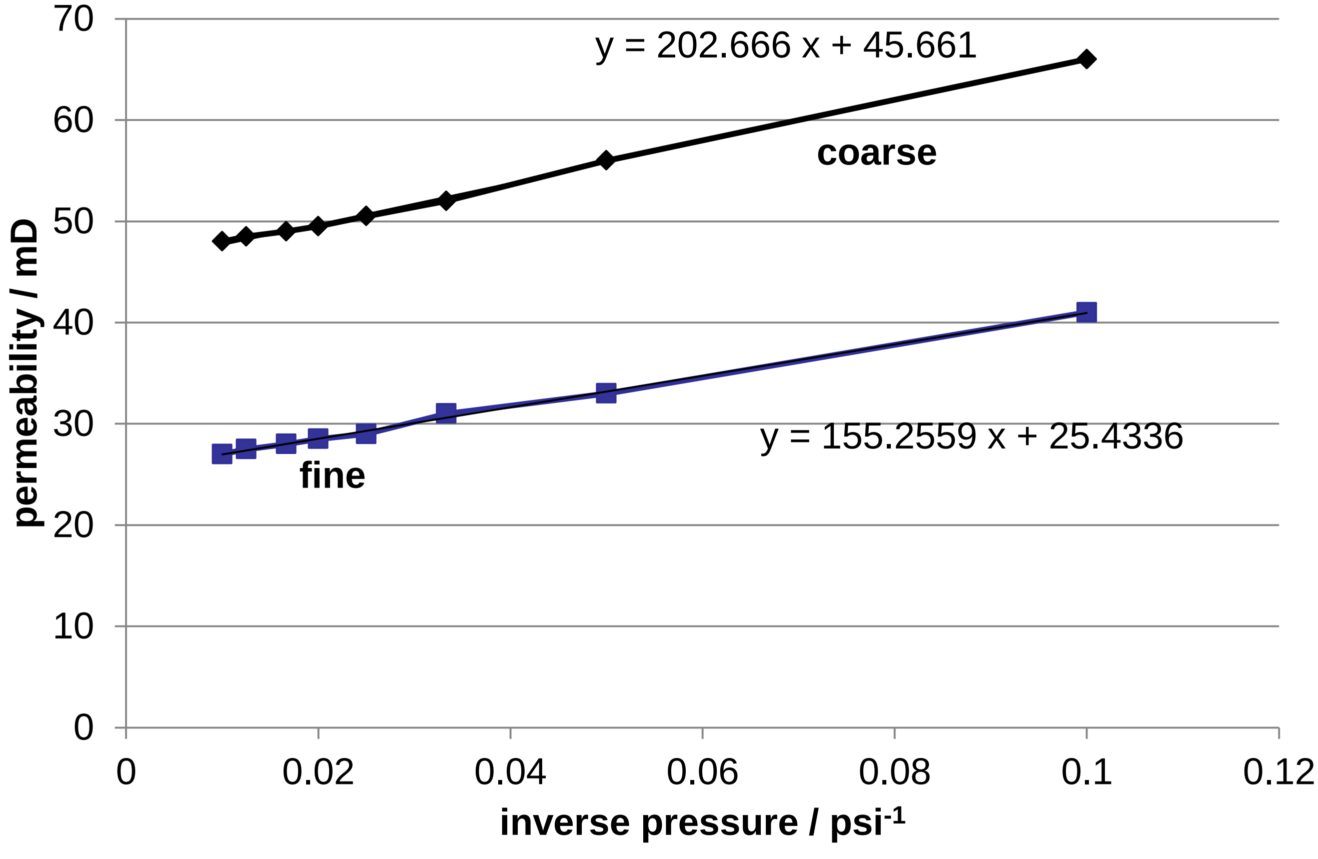
Slip factor

At low gas pressures the mean free path of the gas molecules, i.e., the length of a path that a molecule can travel without colliding to another molecule becomes of the order or large than the pore radius. This was first figured out by Klinkenberg (1941)

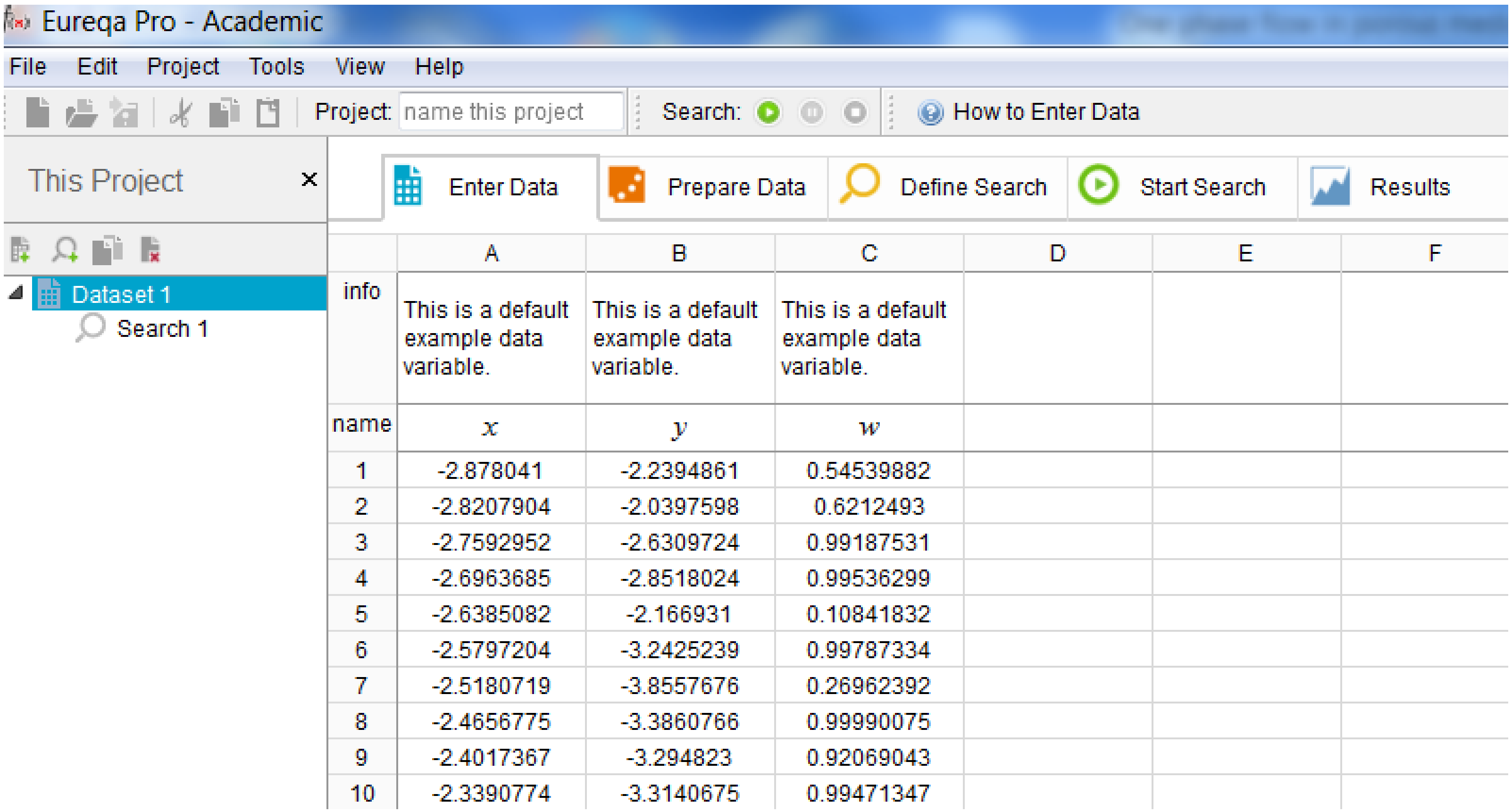
$$k_g = k_l(1 + \frac{4c\lambda}{r}) = k_l(1 + \frac{b}{p}) \tag{31}$$

where k_g is the gas permeability and k_l is the liquid permeability and λ is the mean free path, c =proportionality factor of ≈ 1, and r = radius tube [m]. We call b the slip factor.

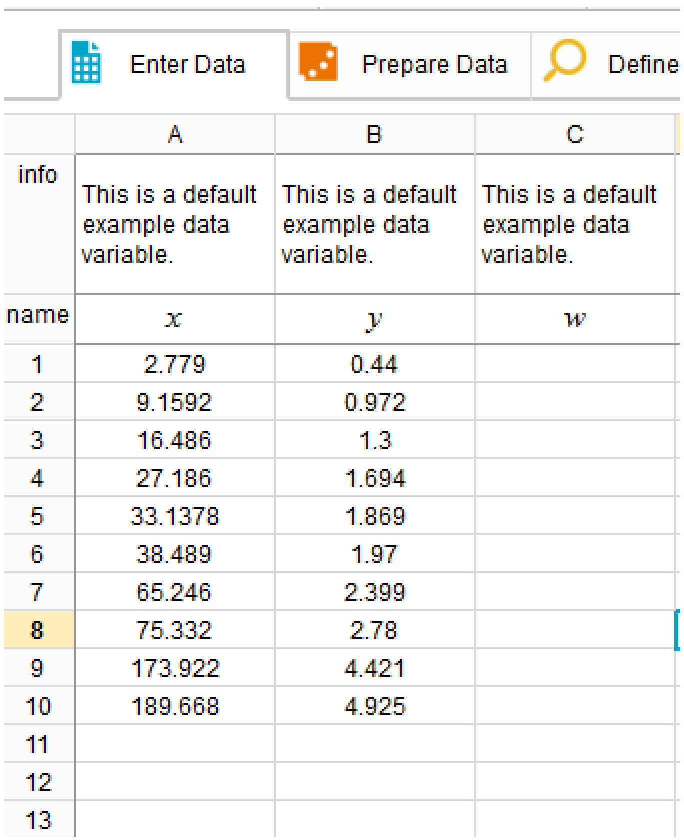
Graphical representation for Klinkenberg factor



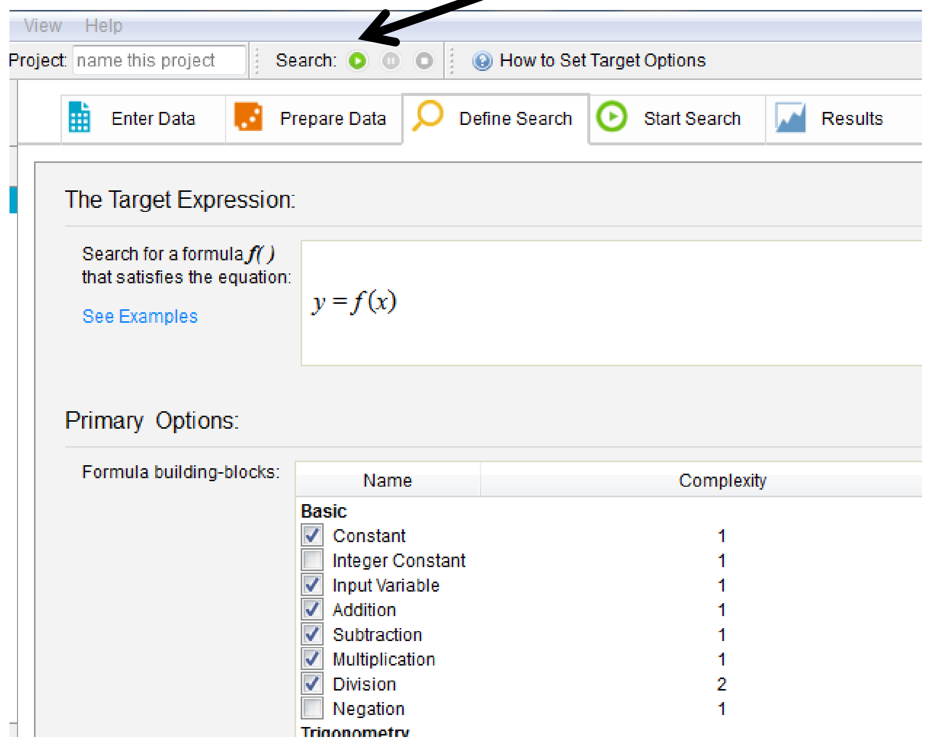
http://www.nutonian.com/products/eureqa/



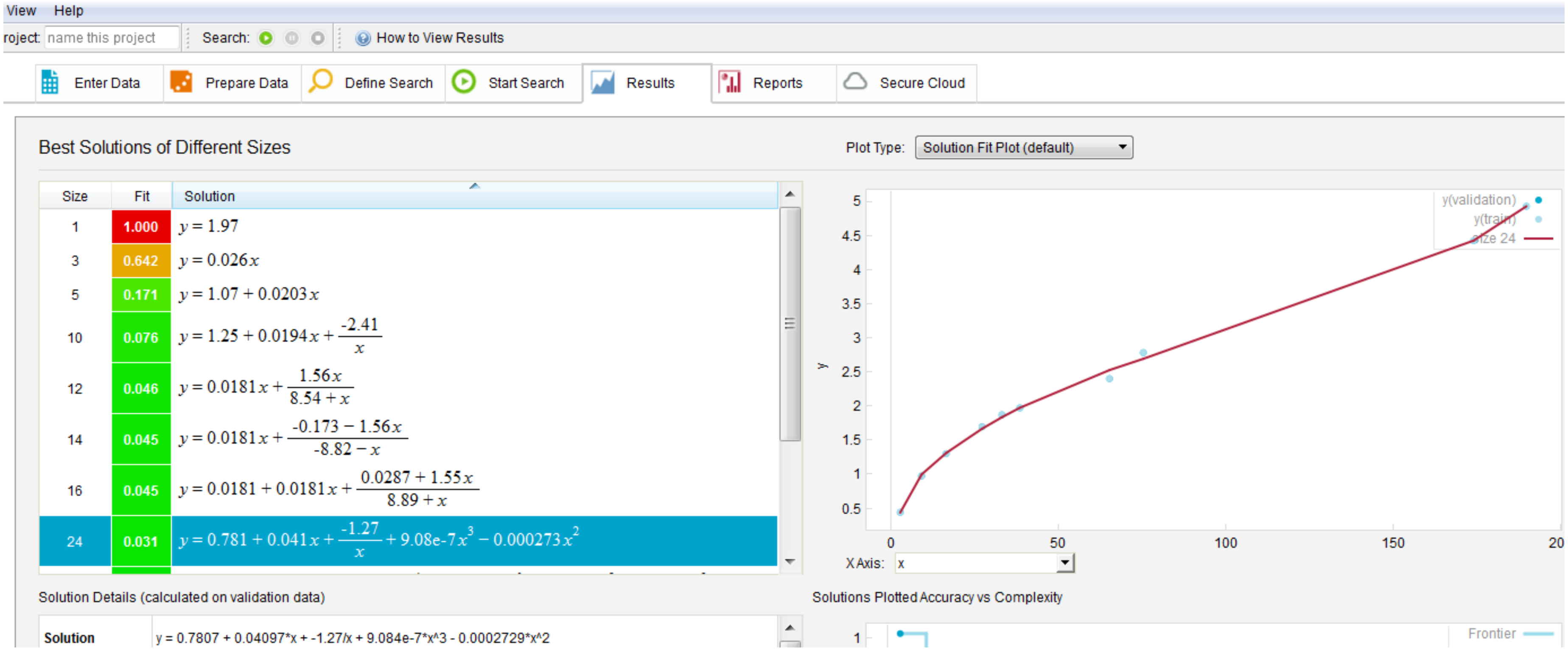
Experimental data inertia II
Enter Data, Define Search, Search


Enter Data | Prepare Data | Define

	A	B	C
info	This is a default example data variable.	This is a default example data variable.	This is a default example data variable.
name	x	y	w
1	2.779	0.44	
2	9.1592	0.972	
3	16.486	1.3	
4	27.186	1.694	
5	33.1378	1.869	
6	38.489	1.97	
7	65.246	2.399	
8	75.332	2.78	
9	173.922	4.421	
10	189.668	4.925	
11			
12			
13			



Results

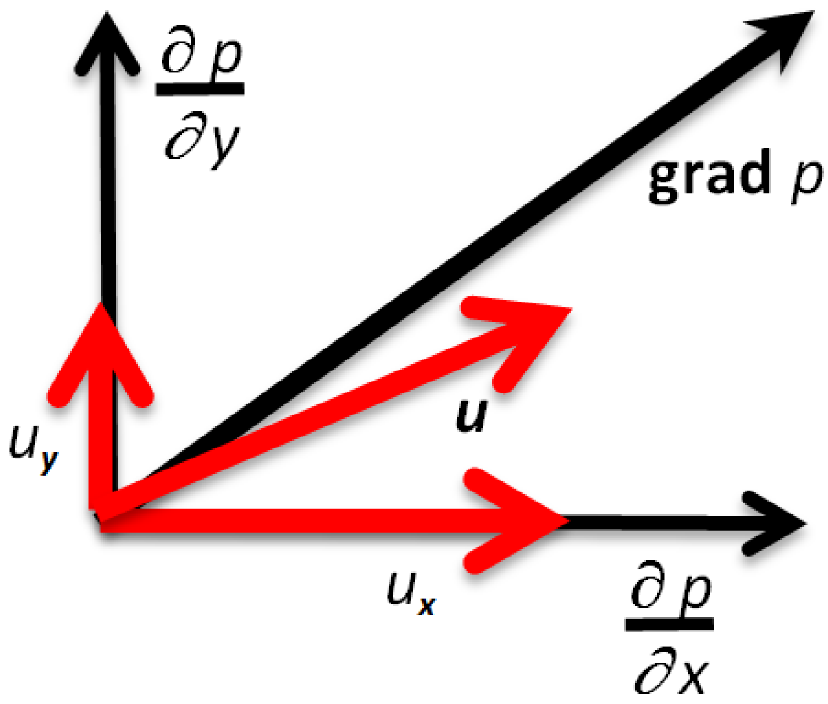

View Help
roject: name this project
Search:
How to View Results
Enter Data
Prepare Data
Define Search
Start Search
Results
Reports
Secure Cloud
Best Solutions of Different Sizes
Plot Type: Solution Fit Plot (default)
Size Fit Solution
1 1.000 y = 1.97
3 0.642 y = 0.026x
5 0.171 y = 1.07 + 0.0203x
10 0.076 y = 1.25 + 0.0194x + -2.41/x
12 0.046 y = 0.0181x + 1.56x/(8.54 + x)
14 0.045 y = 0.0181x + (-0.173 − 1.56x)/(-8.82 − x)
16 0.045 y = 0.0181 + 0.0181x + (0.0287 + 1.55x)/(8.89 + x)
24 0.031 y = 0.781 + 0.041x + -1.27/x + 9.08e-7x^3 − 0.000273x^2
y(validation)
y(train)
Size 24
X Axis: x
Solution Details (calculated on validation data)
Solution y = 0.7807 + 0.04097*x + -1.27/x + 9.084e-7*x^3 - 0.0002729*x^2
Solutions Plotted Accuracy vs Complexity
Frontier

Anisotropy

The permeability can be different in different directions, i.e., we have a permeability k_x in the x-direction, a permeability k_y in the y-direction and a permeability k_z in the z-direction. Hence also the mobilities $\lambda = k/\mu$ i.e., the permeability divided by the viscosity can be different in different directions. The mobility can be considered as a tensor.

$$\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = -\begin{pmatrix} \lambda_{xx} & 0 & 0 \\ 0 & \lambda_{yy} & 0 \\ 0 & 0 & \lambda_{zz} \end{pmatrix} \begin{pmatrix} \frac{\partial \phi}{\partial x} \\ \frac{\partial \phi}{\partial y} \\ \frac{\partial \phi}{\partial z} \end{pmatrix} . \tag{33}$$

Anisotropy 2



The shown pressure gradient **grad** p has equal components in the x-direction and in the y-direction. The permeability in the y-direction is smaller than in the x-direction. Hence the Darcy velocity u_y in the y-direction is smaller than the Darcy velocity u_x in the x-direction. Therefore the total velocity **u** has not the same direction as **grad** p

Mobility tensor

Darcy velocity vector has a different direction than the potential gradient. In general we have:

$$\begin{pmatrix} u_x \\ u_y \\ u_z \end{pmatrix} = - \begin{pmatrix} \lambda_{xx} & \lambda_{xy} & \lambda_{xz} \\ \lambda_{yx} & \lambda_{yy} & \lambda_{yz} \\ \lambda_{zx} & \lambda_{zy} & \lambda_{zz} \end{pmatrix} \begin{pmatrix} \frac{\partial \phi}{\partial x} \\ \frac{\partial \phi}{\partial y} \\ \frac{\partial \phi}{\partial z} \end{pmatrix} . \qquad (34)$$

Calculation of permeability tensor

Ignoring gravity terms we can write Darcy's law as $\mathbf{u} = \mathbf{k} \cdot \nabla \mathbf{p}/\mu$. If we apply the symmetry operator to this equation we obtain $\mathbf{R} \cdot \mathbf{u} = 1/\mu \quad \mathbf{R} \cdot \mathbf{k} \cdot \mathbf{R}^{-1} \cdot \mathbf{R} \cdot \nabla \mathbf{p}$.
Therefore we obtain for $\mathbf{k}$

$$\mathbf{k} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} k_{//} & 0 \\ 0 & k_\perp \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} \tag{4.29}$$

$$\mathbf{k} = \begin{bmatrix} \cos^2\theta \; k_{//} + \sin^2\theta \; k_\perp & \cos\theta \sin\theta \; (k_{//} - k_\perp) \\ \cos\theta \sin\theta \; (k_{//} - k_\perp) & \cos^2\theta \; k_\perp + \sin^2\theta \; k_{//} \end{bmatrix} \tag{4.30}$$

4.4.1 Exercise VIII

Use matrix multiplication in EXCEL to validate Eq. 4.30. Take $k_{//} = 10$ and $k_\perp = 1$ and choose an angle. Use the EXCEL help function (F1) to obtain the procedure how to use "MMULT".

Mass balance

The mass conservation equation reads that the accumulation of mass $\frac{\mathrm{d}m}{\mathrm{d}t}$ equals the net inflow of mass via the boundary S

$$\frac{\mathrm{d}m}{\mathrm{d}t} = -\oint_S \rho\mathbf{u}.\mathbf{n}dS \; . \tag{35}$$

In this equation is u the specific discharge. For stationary situations the LHS is zero. Application of the divergence theorem (Integral theorem of Gauss) leads to

$$\oint_S \rho\mathbf{u}.\mathbf{n}dS = \int_V \mathbf{div}\rho\mathbf{u}dV = 0 \; , \tag{36}$$

Darcy's law + mass balance

$$\mathbf{div}\ (\rho \mathbf{u}) = 0\ . \tag{37}$$

Substitute Darcy's law

$$\mathbf{div}\ (\rho \mathbf{u}) = \mathbf{div}\left(\frac{-k\rho}{\mu}\mathbf{grad}\ \ (P + \rho g z)\right) = 0\ . \tag{38}$$

If ρ is constant we can simplify to

$$\mathbf{div}\left(\frac{k}{\mu}\mathbf{grad}\ \ (P + \rho g z)\right) = \mathbf{div}\left(\frac{k}{\mu}\mathbf{grad}\ \ (\phi)\right) = 0\ . \tag{39}$$

In hydrology we would use the notation

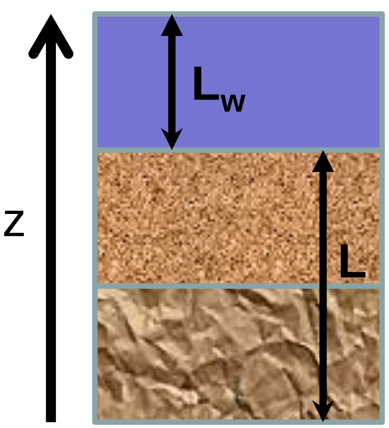
$$\mathbf{div}\ \mathbf{u} = \mathbf{div}\left(\frac{-k\rho g}{\mu}(\mathbf{grad}\ (\frac{P}{\rho g} + z)\right) = -\mathbf{div} K\ \mathbf{grad}\ h = 0\ . \tag{40}$$

1D flow problem

The model equations for a single phase flow can be derived by substitution of Darcy's Law ionto the mass balance equation. We take z as pointing vertically upward. We substitute Darcy's law $u = -\frac{k}{\mu}\left(\frac{dp}{dz} + \rho g\right) = -\frac{k}{\mu}\frac{d}{dz}(p + \rho g z) = -\frac{k}{\mu}\frac{d\phi}{dz}$ into the mass balance equation for incompressible flow in $1 - D$: $\frac{du}{dz} = 0$ and obtain

$$\frac{d}{dz}\left(\frac{k}{\mu}\frac{d\phi}{dz}\right) = 0 \,. \tag{3.1}$$

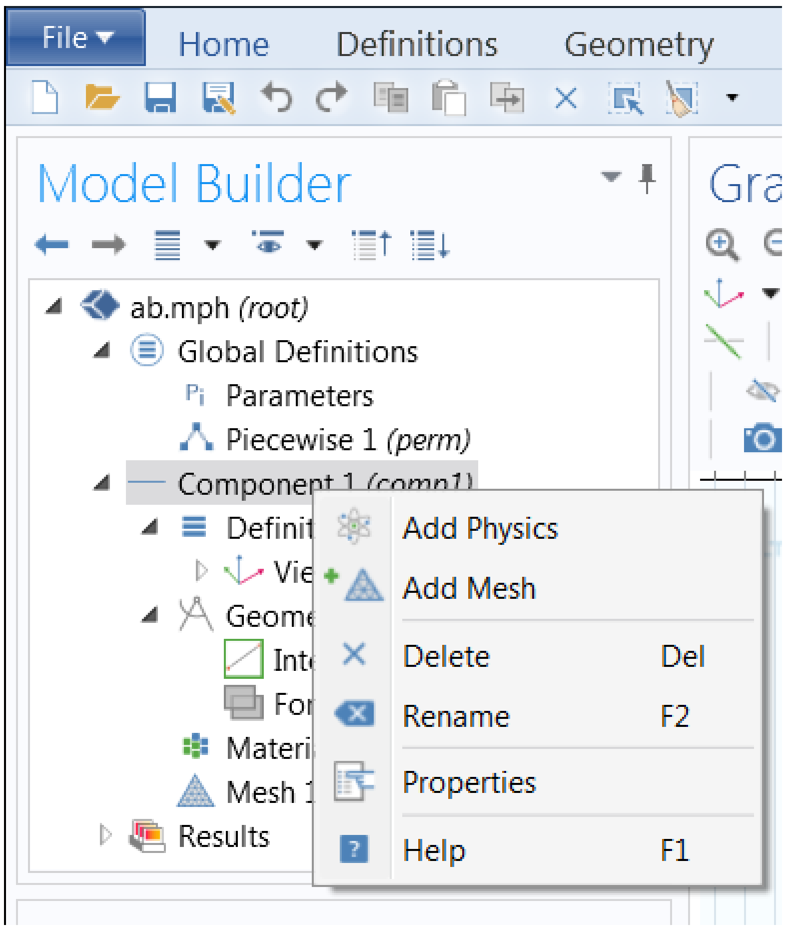
where we have the boundary condition that at $z = 0$, $p = 0$ and hence also $\phi = 0$ and at $z = L$ the pressure is $p(z = L) = \rho_w g L_w$ and thus $\phi = \rho_w g L_w + \rho_w g L$.

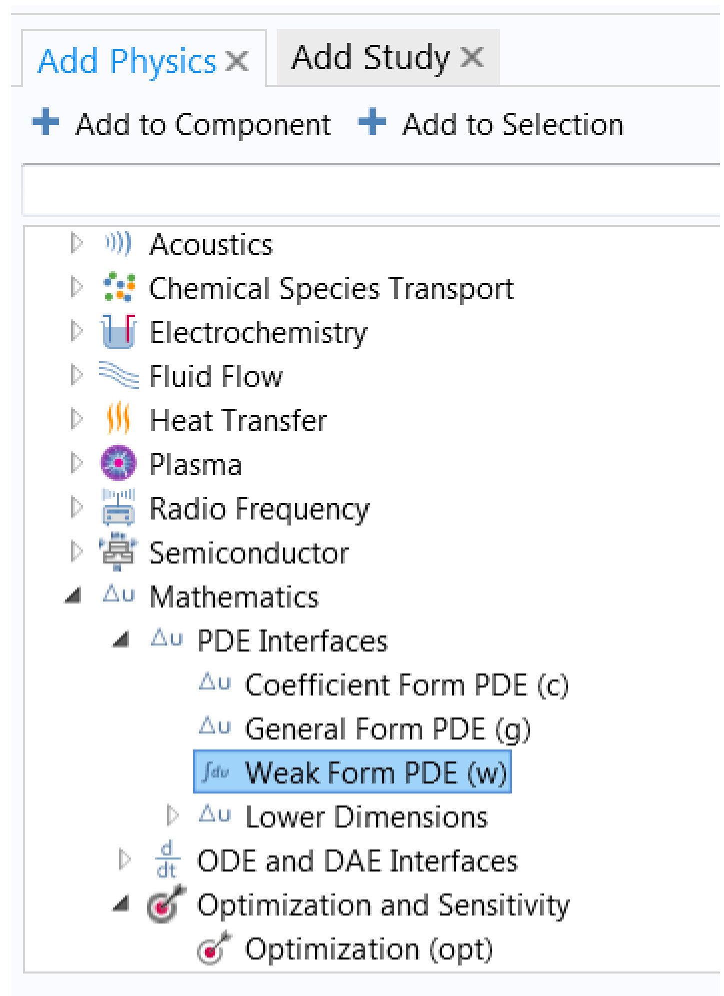


$\phi = \rho_w\, g(L + L_w)$

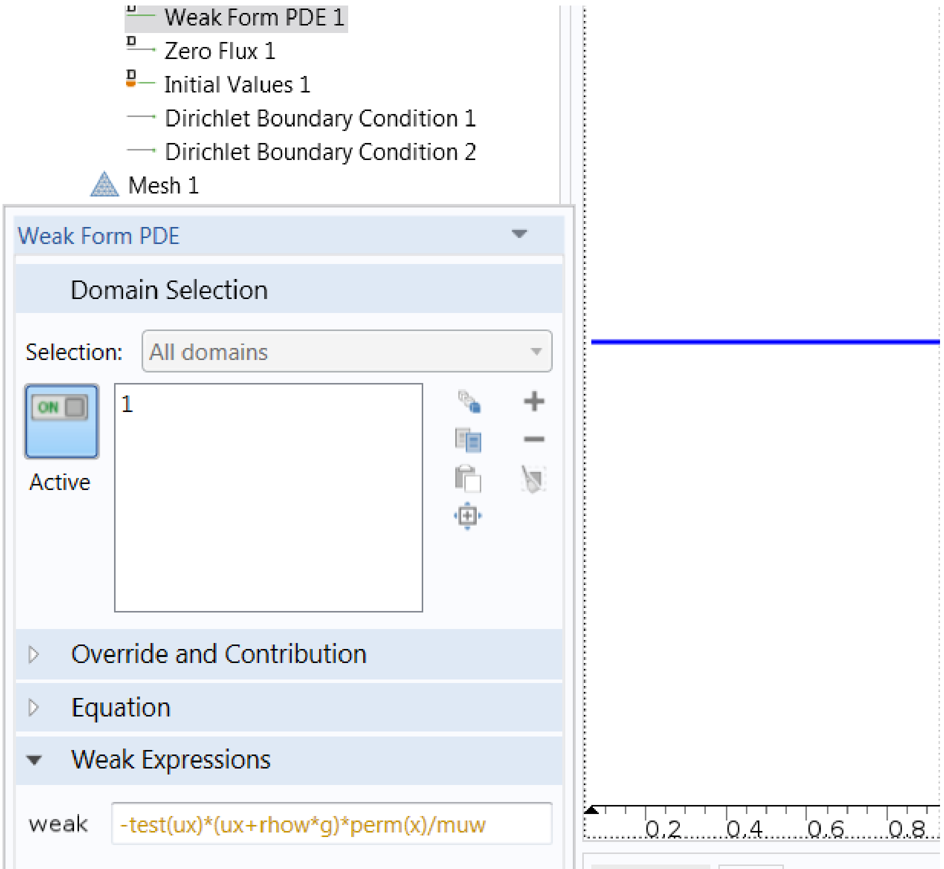
$\phi = 0$

Right click "Components" → Add Physics → Weak Form PDE (w) → Add to Component





Click: “Weak Form PDE (w)” → Right Click: “Weak Form PDE 1”

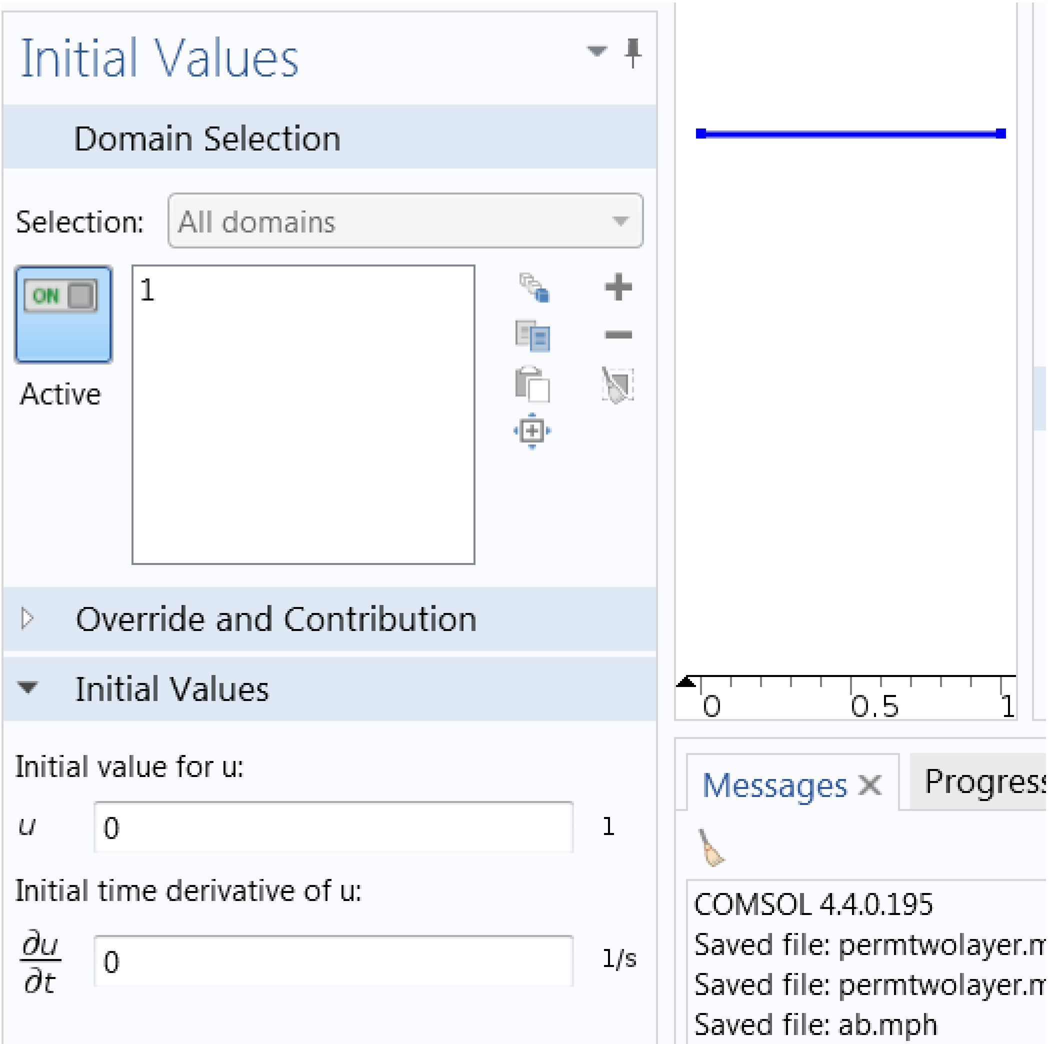


Put in Equation in weak:

- test(ux)*(ux+rhow*g) * perm(x)/muw

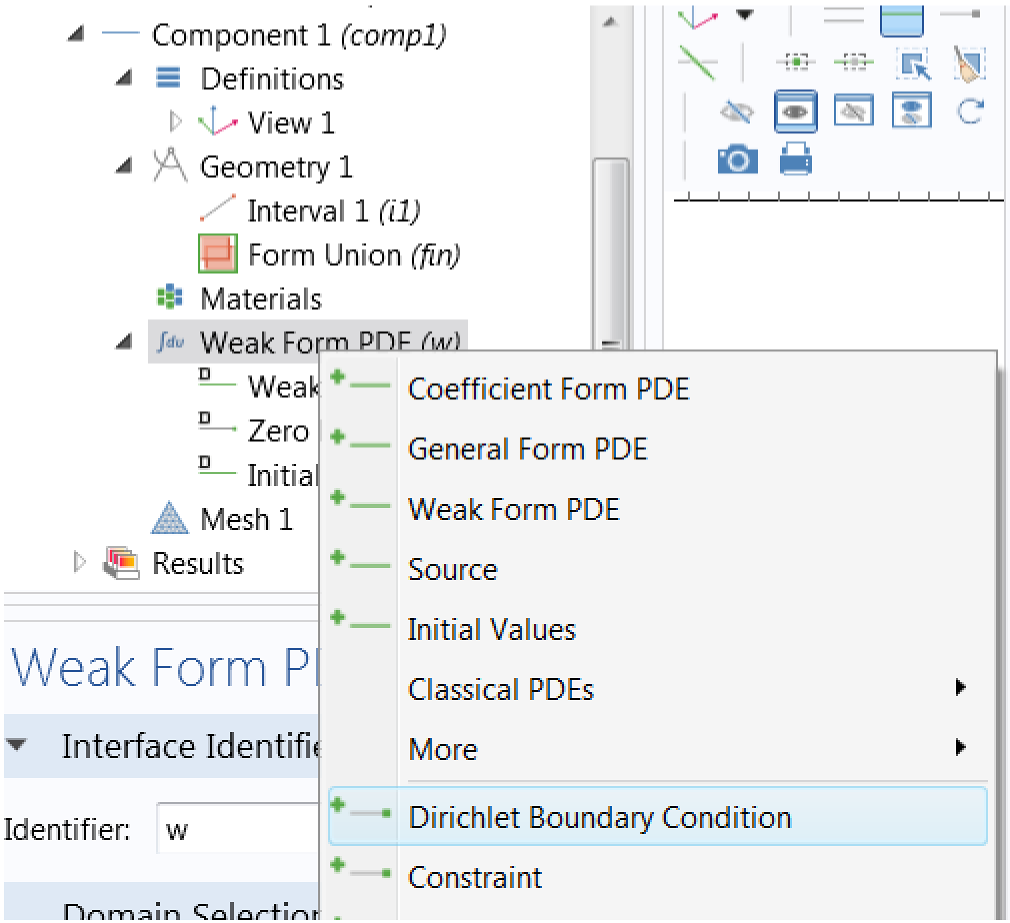
Click on the line to make sure that a “1”appears in the square box; otherwise click on the box above Active

Click: “Initial Values”



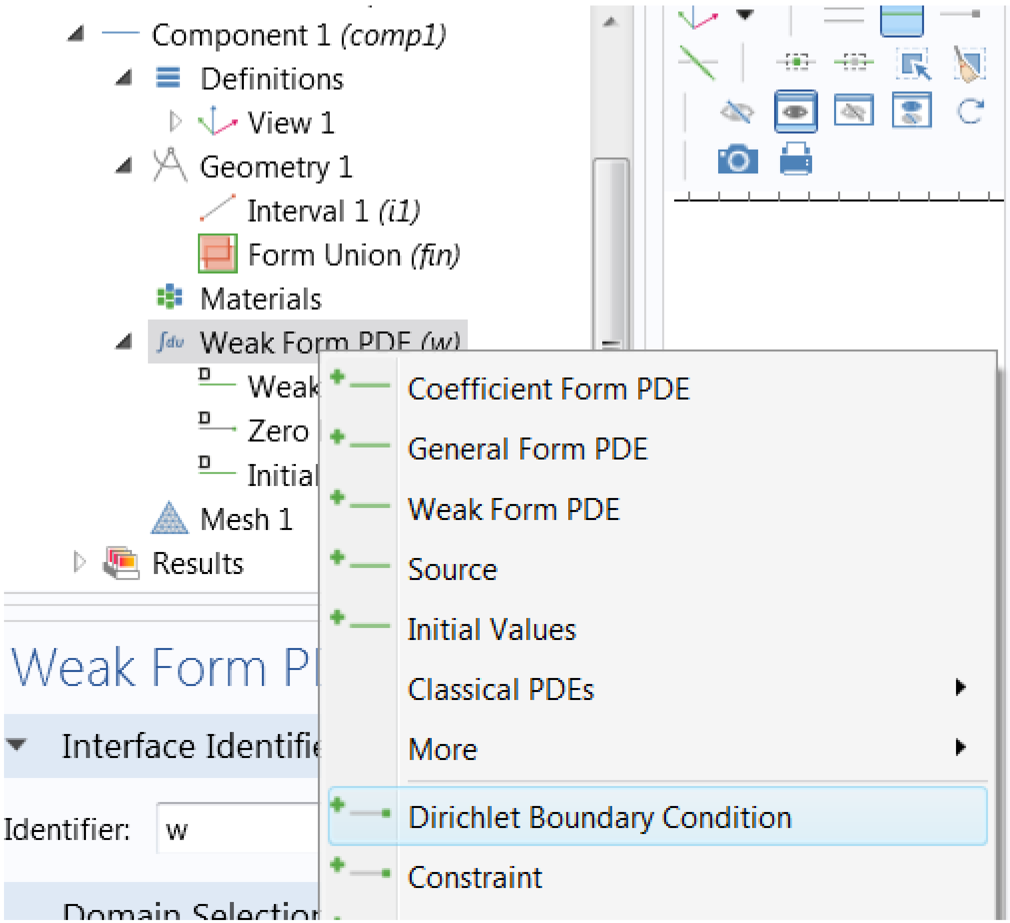
Click on the line to make sure that a “1”appears in the square box; otherwise click on the box above Active

Right Click: "Weak form of PDE (w)"



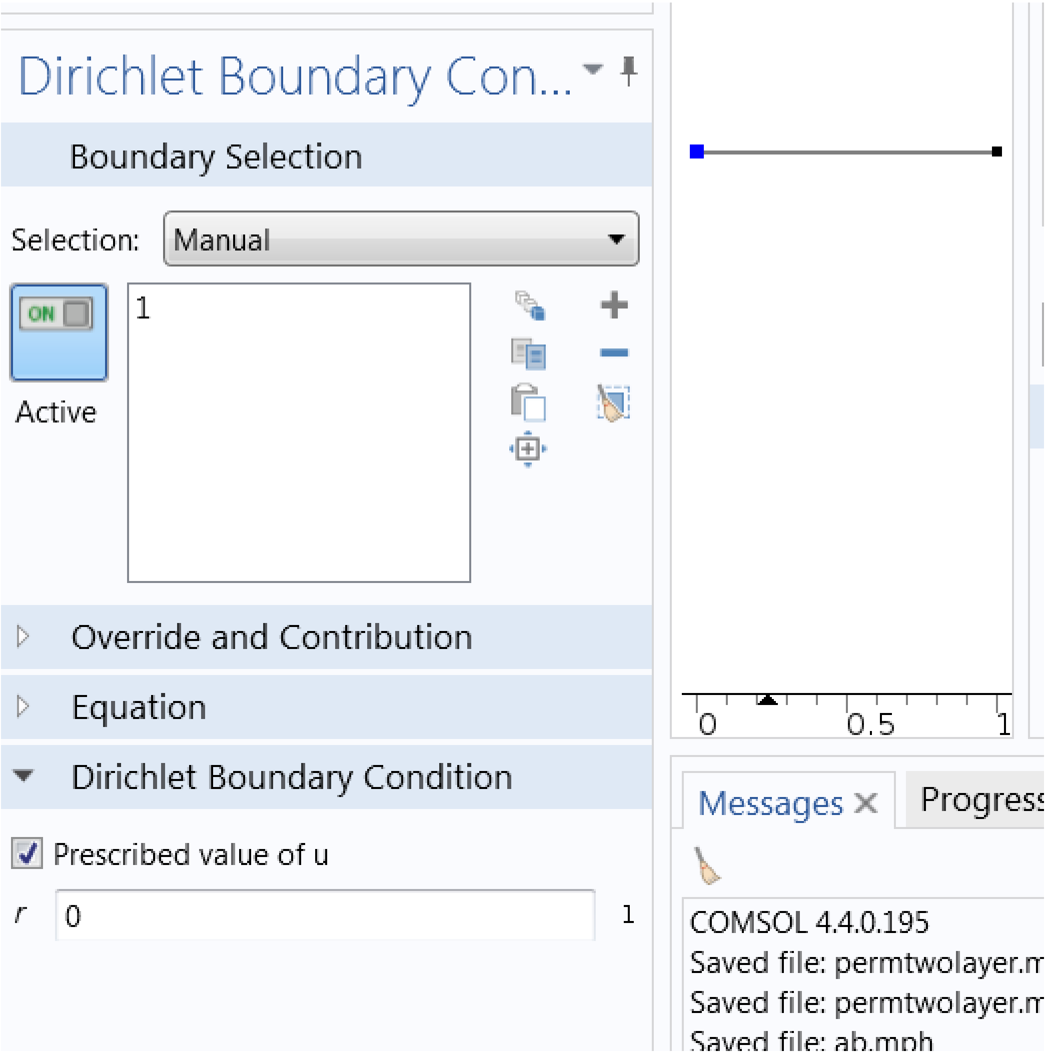
Choose Dirichlet Boundary Condition

Right Click: "Weak form of PDE (w)"



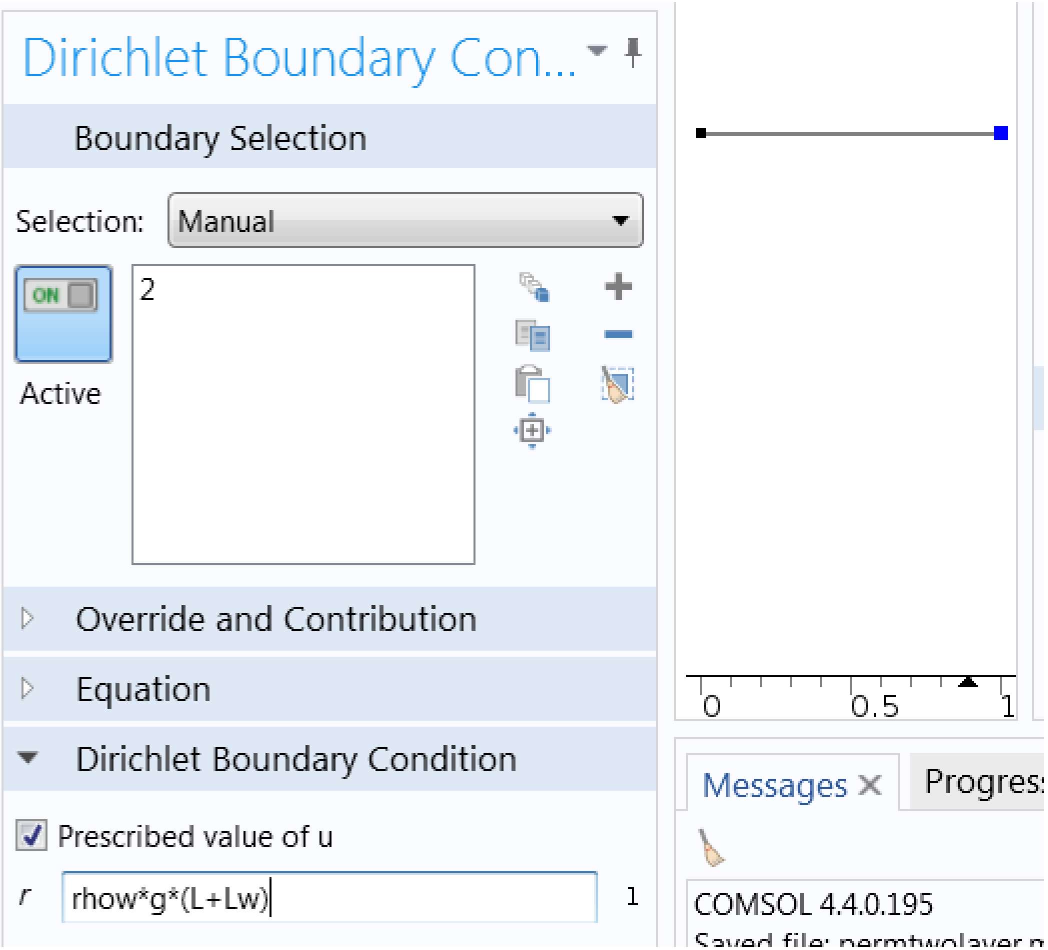
Choose Dirichlet Boundary Condition

Click: "Dirichlet Boundary Condition"



Click on left boundary point such that a "1" appears in the box
Assign the value zero to this point

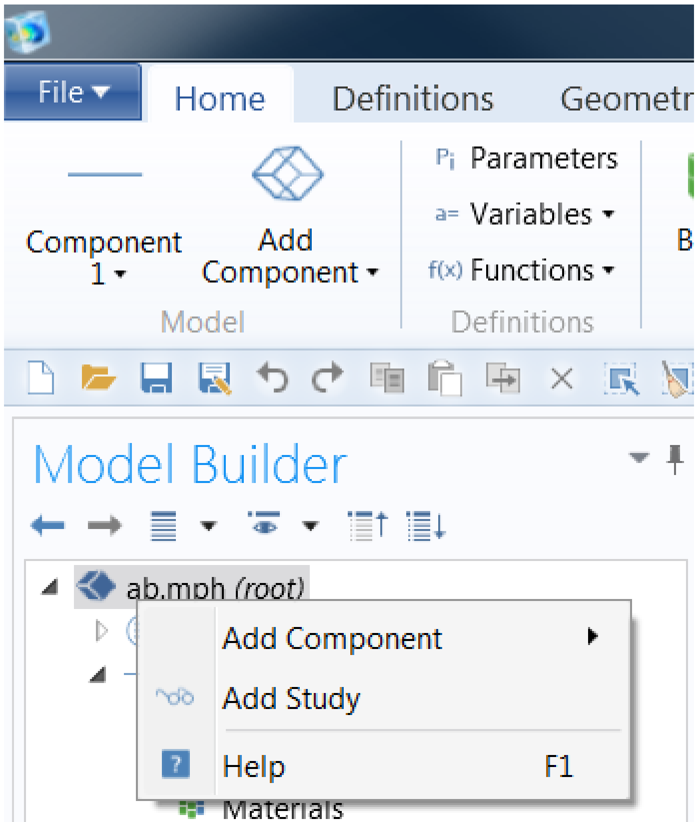
Click: “Dirichlet Boundary Condition”

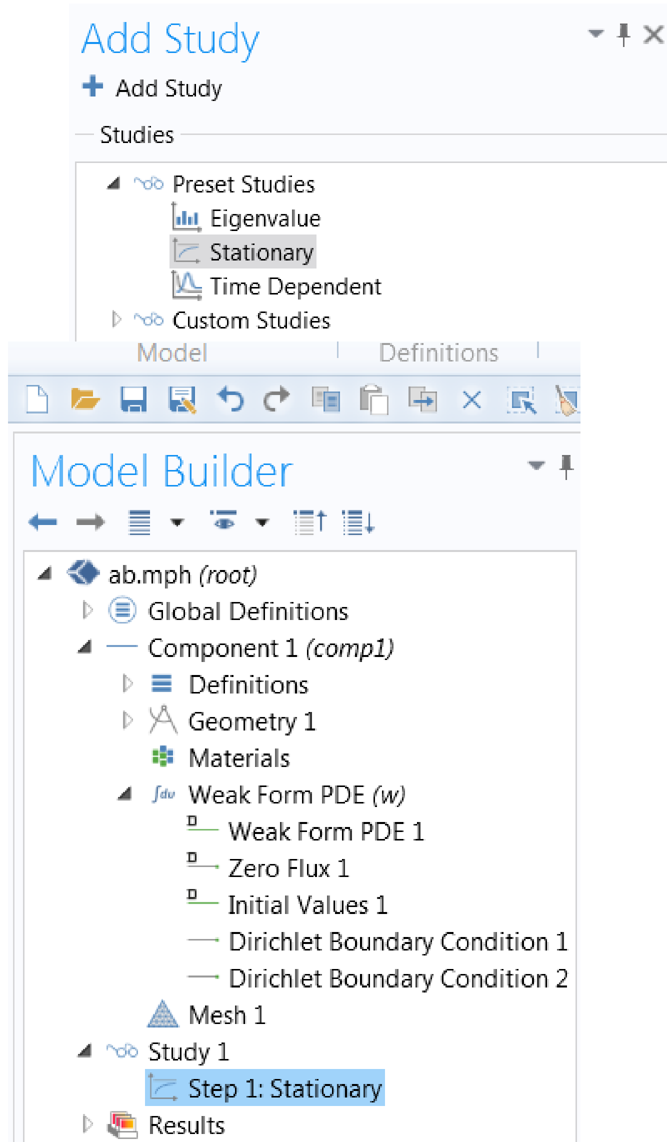


Now put in box r = rhow*g*(L+Lw)

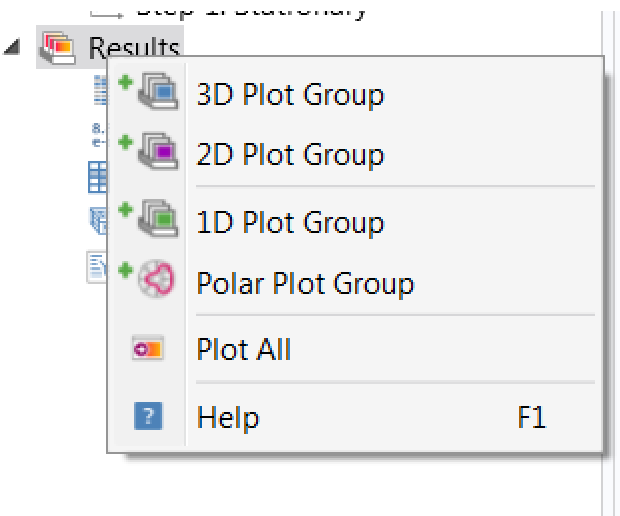
Click on right boundary point such that a “2” appears in the box

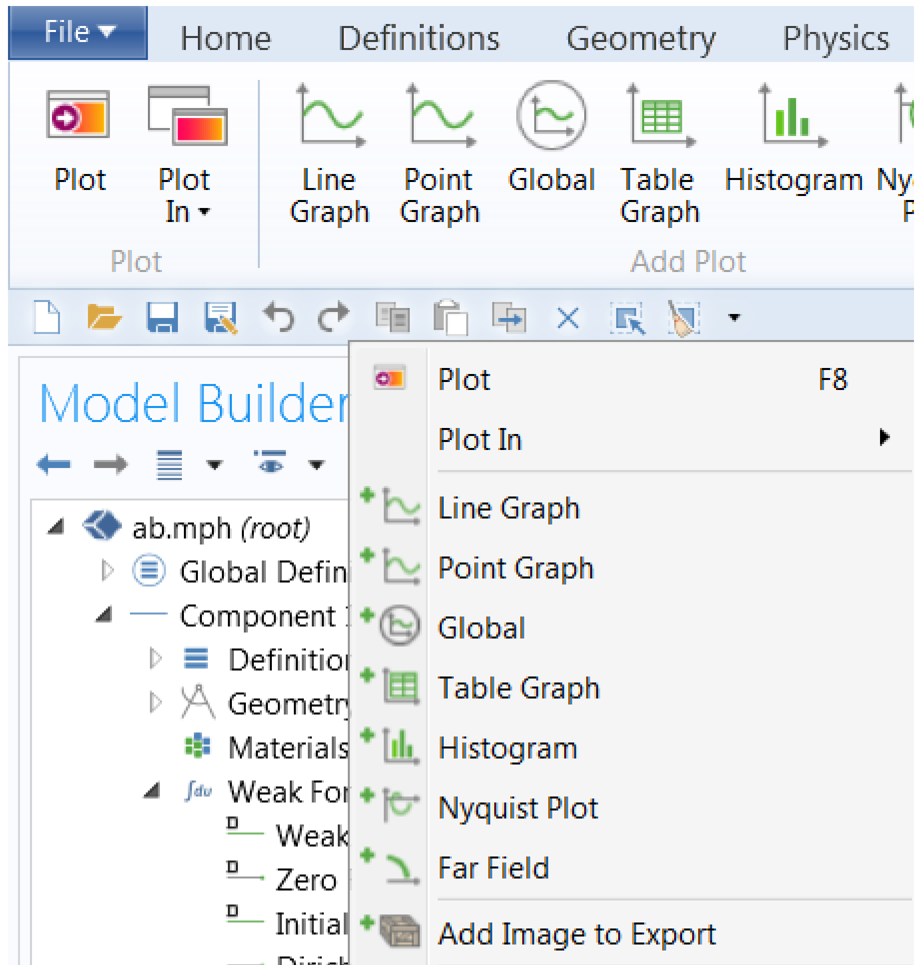
Right Click: “ab.mph”
Click: stationary + Add study





Right Click: “Results”
Right Click: “1D plot group”
Click Line Graph





Weak form

We like to use the weak form because understanding the weak form also leads to better understanding of how the finite element method is implemented in COMSOL Multiphysics. Sometimes the equation is already built in COMSOL Multi-physics and you do not need to know about the weak form. With the built in equation, which you get by choosing "coefficient (general form) PDE", you need to assign zero coefficients to the terms that are not appearing in the equation. It is therefore likely, but not certain, that the weak form does not consider the zero terms and is therefore more efficient. In exceptional cases you can also define problems that are not considered by the templates by the "coefficient (general form) PDE". For educational purposes, it is important to note that the weak form is closer to the finite element implementation, where the test function (to be defined below) is replaced by a basis function (e.g., a tent function).

Weak from II

As said above we will use the weak formulation. We start with equation 3.1 and multiply by a test function ψ. The test function is of compact support, i.e. is non-zero on a finite domain. All its derivatives are continuous, inclusive at the transition of the non-zero values and its boundary at zero. Such a function indeed exists; $\exp -1/x$ is zero and has derivatives zero at $x = 0$. Polynomial functions , e.g., ax^n do not satisfy this condition as its n^{th} derivative is non-zero at $x = 0$.

$$\int \frac{d}{dz}\left(\frac{k}{\mu}\frac{d\phi}{dz}\right)\psi \mathrm{d}z = 0 \; . \tag{3.10}$$

After integration by parts one finds

$$\left(\frac{k}{\mu}\frac{d\phi}{dz}\psi\right)_b - \int \frac{k}{\mu}\frac{d\phi}{dz}\frac{d\psi}{dz}\mathrm{d}z = 0 \; . \tag{3.11}$$

Due to the compact support the boundary integral is zero and we find

$$-\int \frac{k}{\mu}\frac{d\phi}{dz}\frac{d\psi}{dz}\mathrm{d}z = 0 \; . \tag{3.12}$$

In general the weak formulation uses one less differentiation and puts the differentiation on the test function. Hence we use as equation "-test(ux)*ux*perm(x)/muw", where u represents ϕ, ux the derivative of ϕ, i.e., $\frac{d\phi}{dz}$ and "test(ux)" represents the derivative of the test function $\frac{d\psi}{dz}$.

UPSCALING

Arithmetic, harmonic and geometric Averages

$$k_{\mathrm{h}} = \sum_{i=1}^{\mathrm{N}} \frac{\mathrm{k}_i \mathrm{h}_i}{\mathrm{H}}, \quad k_{\mathrm{h}} = \frac{1}{H} \int_0^{\mathrm{H}} k dx \ .$$

$$k_v = \frac{1}{\sum_{i=1}^{\mathrm{N}} \frac{\mathrm{h}_i}{\mathrm{k}_i \mathrm{H}}} \quad k_{\mathrm{v}} = \frac{H}{\int_0^{\mathrm{H}} \frac{1}{k} \mathrm{dx}} \ .$$

$$k_{\mathrm{geo}} = \prod_{i=1}^{n} \sqrt[n]{\mathrm{k}_i} \ .$$

Derivation arithmetic/ harmonic

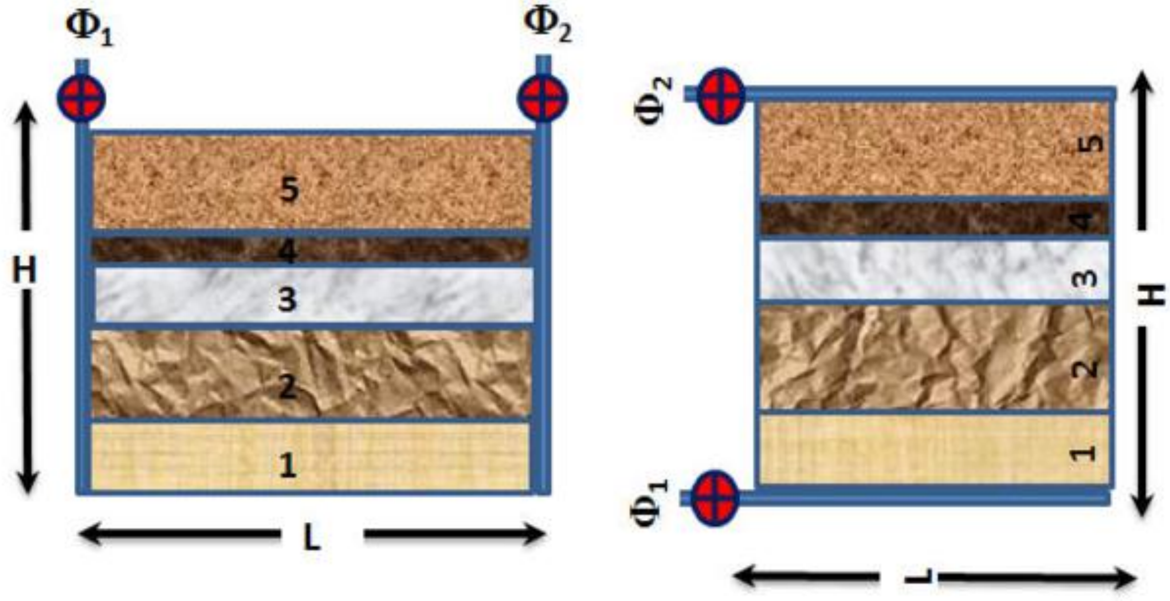


Figure 14: Flow through a stack of horizontal layers with characteristic thickness h_i and permeability k_i with $i = 1, ..., 5$ In both cases the flow is from left to right.

Integration over thickness of layer

$$\frac{\partial}{\partial x}\left(\frac{k}{\mu}\frac{\partial\phi}{\partial x}\right)+\frac{\partial}{\partial y}\left(\frac{k}{\mu}\frac{\partial\phi}{\partial y}\right)+\frac{\partial}{\partial\zeta}\left(\frac{k}{\mu}\frac{\partial\phi}{\partial\zeta}\right)=0\ , \tag{48}$$

where we have replaced z by ζ to indicate that the X-dip direction is not necessarily vertical. The assumption, which is required to get a useful result if we integrate over the coordinate ζ, is that $\phi(x,y,\zeta)\rightarrow\phi_o(x,y)$. In other words we assume that the potential does not depend on ζ. This assumption appears to be reasonable (see [21], page 206) if

$$\sqrt{\frac{k_\zeta}{k_{//}}}\frac{L}{H}>>1\ , \tag{49}$$

Integration over the height

$$\int_0^H \left(\frac{\partial}{\partial x}\left(\frac{k}{\mu}\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{k}{\mu}\frac{\partial \phi}{\partial y}\right) + \frac{\partial}{\partial \zeta}\left(\frac{k}{\mu}\frac{\partial \phi}{\partial \zeta}\right)\right) d\zeta = 0\ . \tag{50}$$

Note that the last term in Eq. (48) drops out upon integration. Moreover the porosity φ and the permeability k are the only quantities that depend on ζ. More over we use the following abbreviations $\overline{k}H = \int_0^H k d\zeta$ and $\overline{\varphi}H = \int_0^H \varphi d\zeta$ Hence we obtain

$$\frac{\partial}{\partial x}\left(\frac{\overline{k}}{\mu}\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{\overline{k}}{\mu}\frac{\partial \phi}{\partial y}\right) = 0\ . \tag{51}$$

Homogenization (under construction)

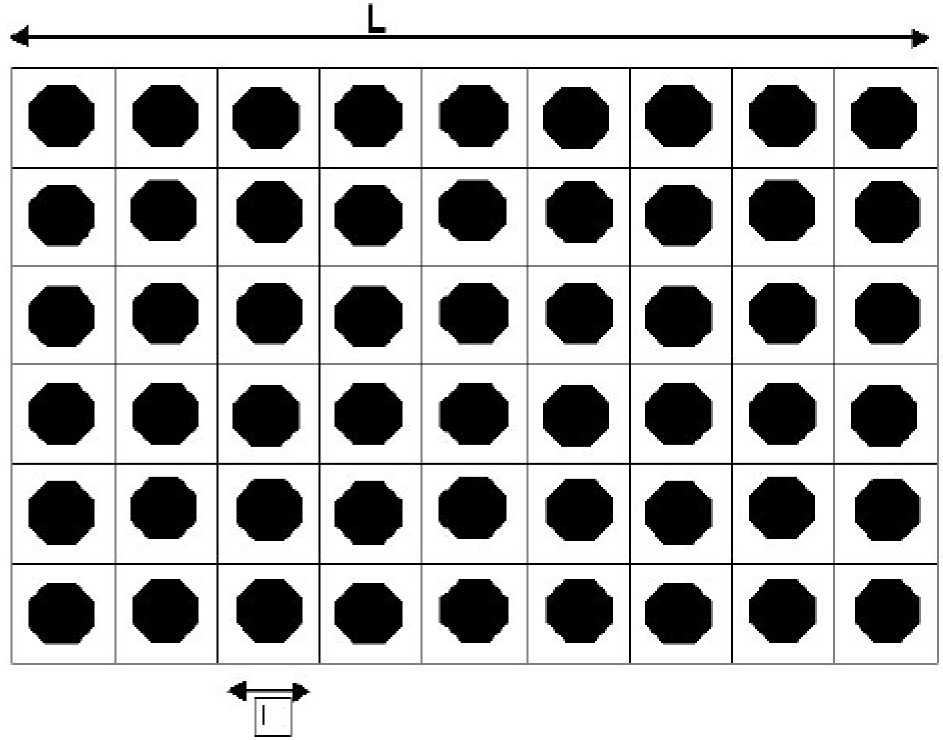


Figure 6: A periodic lattice. Each cell represents a permeability distribution at a small scale. The cell is periodically continued and builds the entire lattice. The length of the entire lattice is L and the length of a single unit cell is l, where $\varepsilon = \frac{l}{L} << 1$.

Procedure

- Take a periodic unit cell that is sufficiently large such that result becomes independent of size
- Subject to periodic boundary discussions

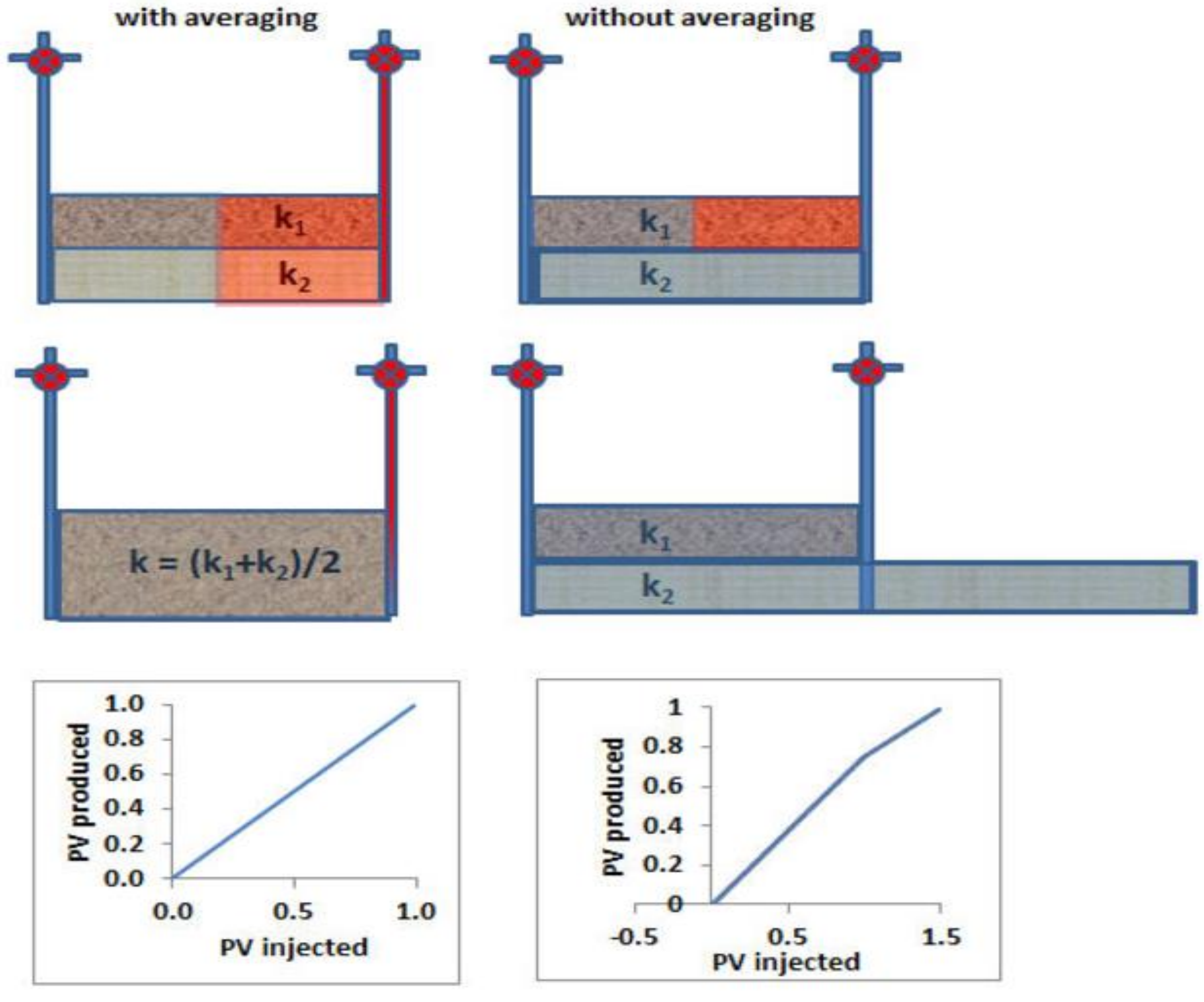
Bourgeat and Piatnitski [7] show that, if separation of scale is possible, effective properties in random media converge as the scale of the unit cell increases, independent of its boundary conditions (periodic, Dirichlet or Neumann).

Effective medium approximation

The effective medium approximation was designed for calculating average resistances in resistor networks. It considers one resistor drawn from a distribution of resistors embedded in a "sea" of average resistances. The equation tells us that the average contribution from all the resistances drawn from the distribution must be zero. For permeabilities with a probability density distribution $h(k)$ the result reads

$$\int_0^\infty h(k) \frac{k - k_{eff}}{k + (\gamma^{-1} - 1)\, k_{eff}} dk = 0 \,, \tag{73}$$

Perfect permeability averaging ≠ perfect simulation



Generation of Random numbers

$$P(\ln k)\mathrm{d}\ln k = \frac{1}{\sqrt{2\pi s^2}}\exp -\frac{(\ln k - \mu)^2}{2s^2}\mathrm{d}\ln k \;, \tag{74}$$

$$P(k)\mathrm{d}k = \frac{1}{\sqrt{2\pi s^2}}\frac{1}{k}\exp -\frac{(\ln k - \mu)^2}{2s^2}\mathrm{d}k \;.$$

where we use the fundamental transformation law of probabilities, i.e.,

$$|p(y)dy| = |p(x)dx|$$

$$p(y) = p(x)|\frac{dx}{dy}| \;. \tag{75}$$

$$\frac{dx}{dy} = p(y) \;. \tag{78}$$

This equation can be integrated to relate the uniformly distributed random number to the cumulative distribution function of y

$$x = \int_{-\infty}^{y} p(y')dy' = F(y) \;,$$

$$y(x) = F^{-1}(x) \;.$$

Generation of random numbers

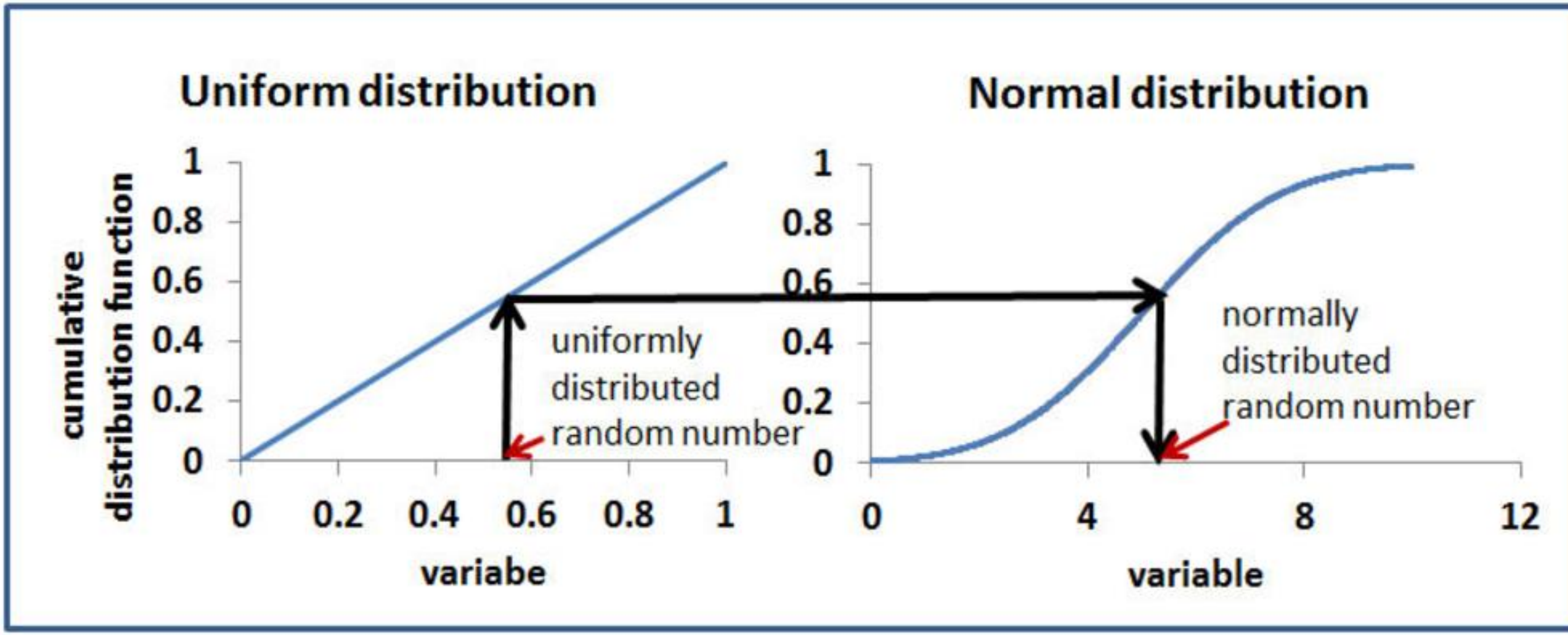


Figure 12: Method to generate a set of normally distributed random numbers with an average of 5 and a standard deviation of 1. Start to generate a uniformly distributed random number and follow the arrows upward to the right and downward to find the normally distributed random number.

Generation of random numbers with EXCEL: $k = \exp(\mu + s^2/2)$ $s = -\ln(1 - V_{DP})$

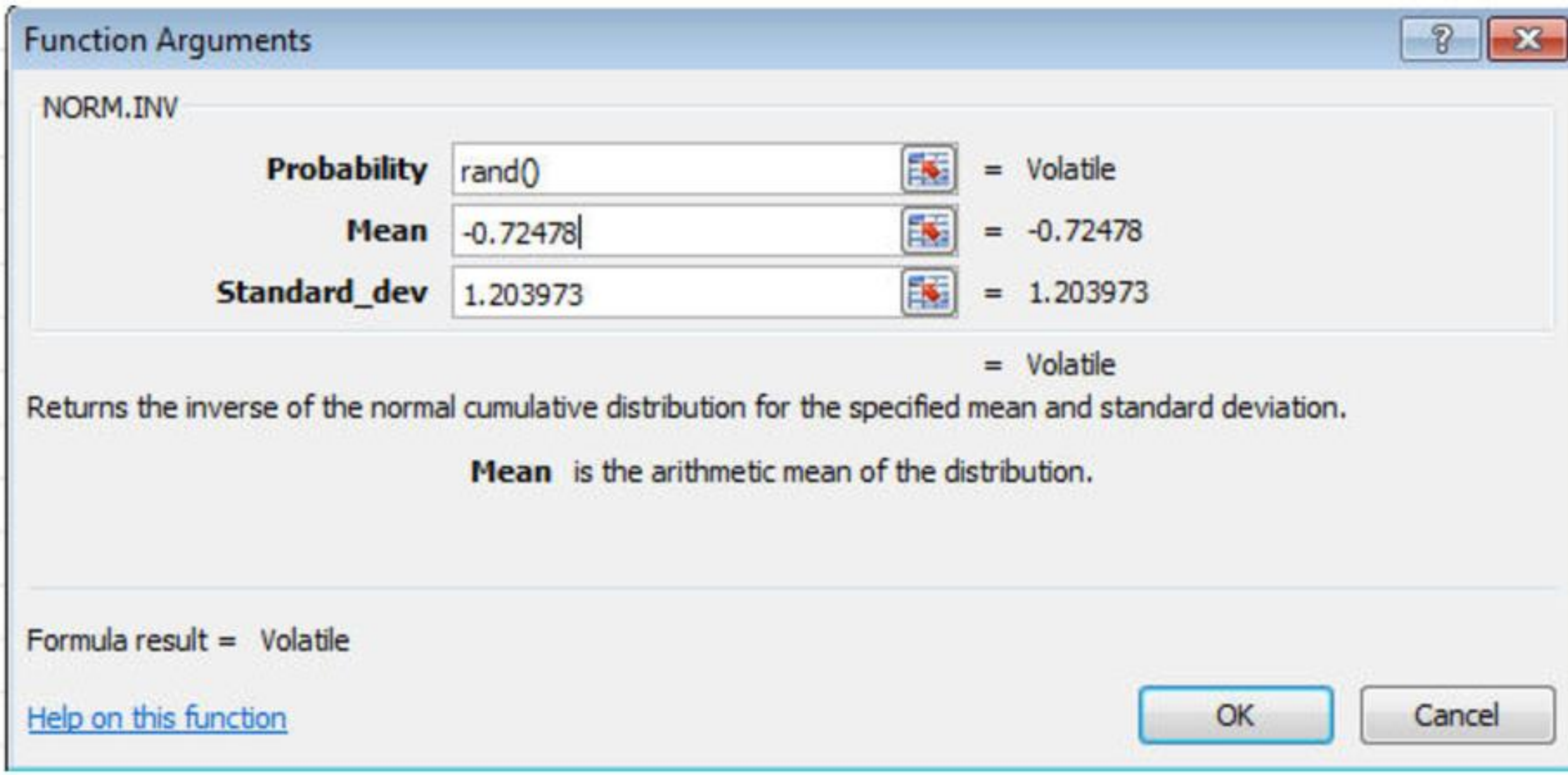


Figure 13: Using the function "norminv" to obtain a normal distribution for $ln(k)$.

Heterogeneity field for COMSOL

- Generate a 27×27 field that can be used in an interpolation function in COMSOL. The field is the exponential of an log-normal field, with an average of one Darcy and a Dykstra-Parson's coefficient of V_{DP}=0.7. Use Eq. (6.4) to calculate s and Eq.(6.3a) to calculate the average of the logarithm of the permeability μ. Use $= EXP(NORMINV(RAND(); mu; s))$. The actual field is a square with length one. The field is periodic, meaning that the first column duplicates the one but last column and that the last column duplicates the the second column. In the same way the top row duplicates the one but last bottom row, whereas the bottom row duplicates the second top row. Start the file by writing %grid in the top corner of an EXCEL file. Do not put a space between % and grid. In the row just below %grid indicate the x-coordinates: -0.02 0.02 0.06 ... 0.98 1.02. In the row below indicate the y-coordinates: -0.02 0.02 0.06 ... 0.98 1.02. Below the coordinate indication indicate %data again without a space between the % and data. Below %data insert the data file. Save as text (Tab delimited). Import the data in COMSOL. Right click "global definitions" $\rightarrow$ functions $\rightarrow$ interpolation. For data source choose, "file", for number of arguments choose "2", for function name choose "kpp". Leave position in file at "1". For data format choose "spreadsheet". For interpolation choose linear and for extrapolation choose constant. Other options are not yet implemented in COMSOL. For arguments choose: "x,y" and for function choose "kpp". Use plot to plot the interpolation function.

Constructing data file for COMSOL

	A	B	C	D	E
4		=B7	=C7	=D7	
5	=D5	=EXP(NORMINV(RAND(),mu,s))	=EXP(NORMINV(RAND(),mu,s))	=EXP(NORMINV(RAND(),mu,s))	=B5
6	=D6	=EXP(NORMINV(RAND(),mu,s))	=EXP(NORMINV(RAND(),mu,s))	=EXP(NORMINV(RAND(),mu,s))	=B6
7	=D7	=EXP(NORMINV(RAND(),mu,s))	=EXP(NORMINV(RAND(),mu,s))	=EXP(NORMINV(RAND(),mu,s))	=B7
8		=B5	=C5	=D5	

	A	B	C	D	E	F	W	X	Y	Z	AA
1	%Grid										
2	-0.02	0.02	0.06	0.1	0.14	0.18	0.86	0.9	0.94	0.98	1.02
3	-0.02	0.02	0.06	0.1	0.14	0.18	0.86	0.9	0.94	0.98	1.02
4	%Data										
5	0.379968	1.213497	0.624017	1.078446	1.673927	0.134171	0.432728	0.928227	0.231804	0.379968	1.213497
6	0.612686	1.833172	0.359985	0.365621	1.256761	0.732938	1.637322	0.304274	0.483216	0.612686	1.833172
7	0.281724	0.271744	0.329308	0.613881	1.061415	0.713174	6.458638	1.684819	0.459933	0.281724	0.271744
8	1.824793	0.693326	1.866567	1.373245	0.472102	1.492567	0.30615	0.858427	2.470346	1.824793	0.693326
9	0.542793	0.31355	0.932172	0.970106	0.157384	0.527931	1.090169	0.27344	0.224412	0.542793	0.31355

	A	B	C	D	E	F	G	H	I	J	K
4	%Data										
5	0.379968	1.213497	0.624017	1.078446	1.673927	0.134171	0.806794	0.509129	3.9251	0.930294	0.987265
6	0.612686	1.833172	0.359985	0.365621	1.256761	0.732938	0.836133	0.857774	0.232448	0.509024	0.523153
7	0.281724	0.271744	0.329308	0.613881	1.061415	0.713174	3.364922	0.592084	0.716084	0.832742	1.701585
8	1.824793	0.693326	1.866567	1.373245	0.472102	1.492567	1.303609	1.242594	1.46735	2.131765	0.959118
9	0.542793	0.31355	0.932172	0.970106	0.157384	0.527931	0.578041	0.176847	1.229545	0.391967	1.616656
29	0.442217	0.285794	0.568836	0.989234	0.305134	6.25373	0.699269	0.316498	0.311142	0.767363	0.836307
30	0.379968	1.213497	0.624017	1.078446	1.673927	0.134171	0.806794	0.509129	3.9251	0.930294	0.987265
31	0.612686	1.833172	0.359985	0.365621	1.256761	0.732938	0.836133	0.857774	0.232448	0.509024	0.523153

Implementation in COMSOL

ut*test(u) + test(ux)*ux*perm(x,y)+test(uy)*uy*perm(x,y)

Use the same procedure for start up as indicated in Fig. 6, but instead of 1-D choose 2-D and instead of stationary choose "time dependent".

- Right click geometry and choose "Square". Choose the side length equal to one and the base corner at $x = 0$, $y = 0$. Use zero rotation angle. Press "build all".
- Choose mesh, physics controlled mesh, extremely fine. Finish mesh implementation by choosing "build all".
- In the "weak form PDE" $\rightarrow$ "weak form PDE" implement: "test(ux)*ux*kpp(x,y) + test(uy)*uy*kpp(x,y)+ut*test(u)".
- Be sure that the interpolation function is defined and named "kpp". As initial condition choose "$u = u_t = 0$. Choose top of "weak form PDE", click on the square and press "+" next to the rectangle to be sure that a "1" appears in the top corner.
- Implement Dirichlet boundary conditions at east and west side and implement periodic boundary conditions at north and south side. Choose again top of "weak form" and right click. A choice of boundary conditions will appear.

PERIODIC AND SEMI-PERIODIC BOUNDARY CONDITIONS BOUNDARY CONDITIONS

Implementation in COMSOL ctd.

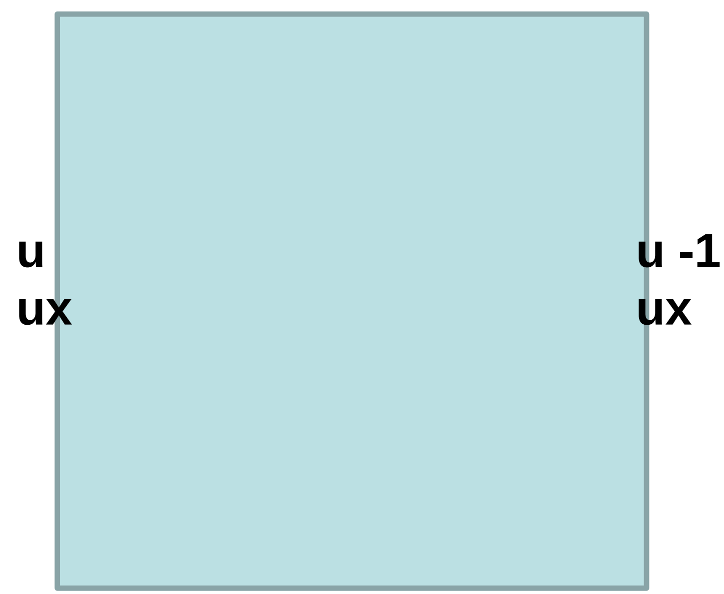
- Implement semi-periodic boundary conditions also at east and west side, meaning that the potential on the west side adds one to the potential on the east side. Hint: use linear extrusion and procedure indicated at the Figures 8.1.1 etc., below. The implementation of this BC is very complicated. "A Linear Extrusion model coupling maps an expression defined on a source domain to an expression that can be evaluated on the destination domain. Use a linear extrusion when the correspondence between evaluation points in the source and destination is linear".

- Right click on "definitions" $\rightarrow$ "probes" $\rightarrow$ "Boundary probe". Click the West-boundary (1) in the rectangle after clicking away (clear selection) all other points. Press curly arrow above the probe settings. Use as expressions "-kpp(x,y)*ux". Again click on "definitions" $\rightarrow$ "probes" $\rightarrow$ "Boundary probe". Click the East-boundary (4) in the rectangle after clicking away (clear selection) all other points. Press curly arrow above the probe settings. The values for the east and west boundary should be the same.

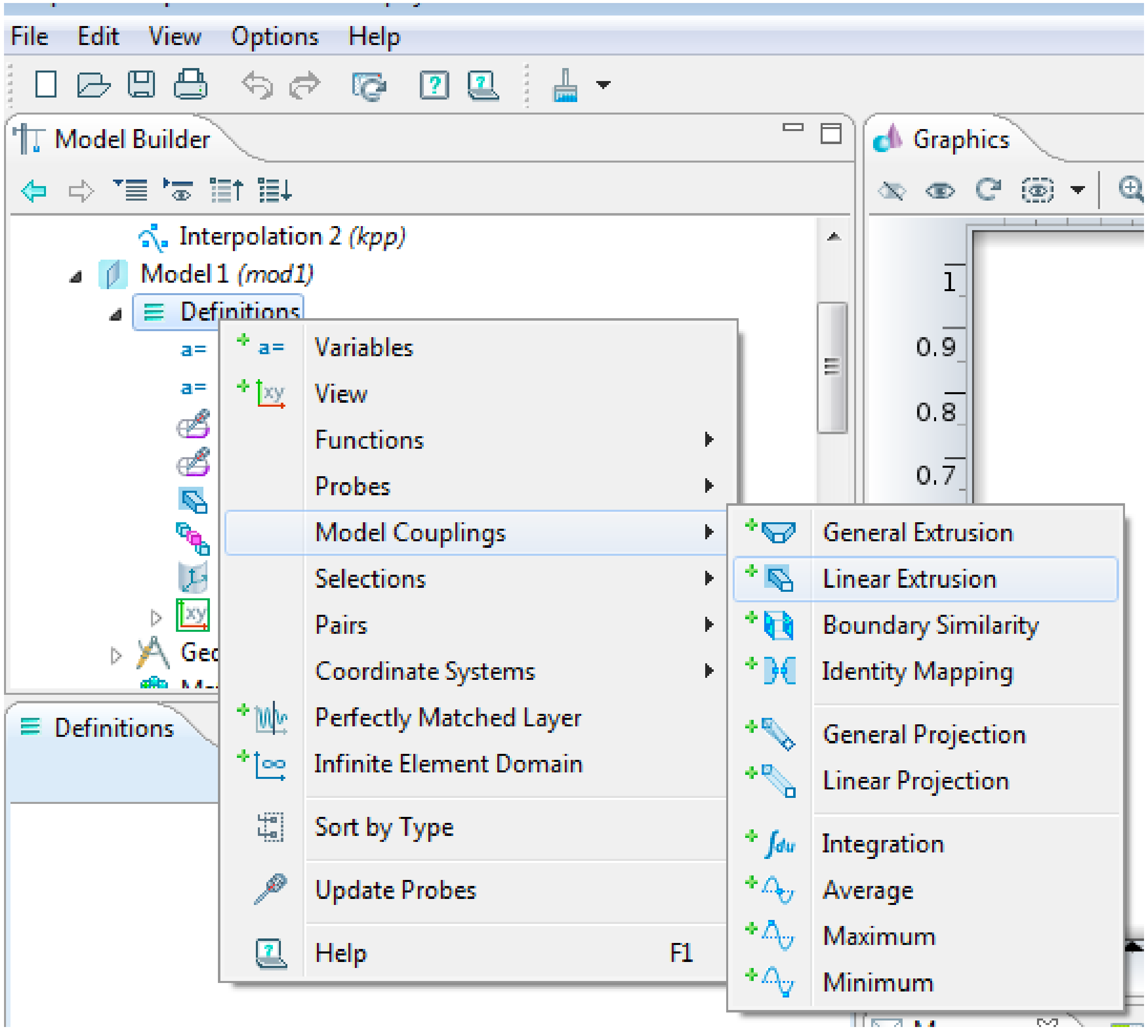
Semi periodic boundary conditions

- The definition of semi-periodic boundary conditions is hopelessly difficult. Still the procedure is mentioned here for easy reference

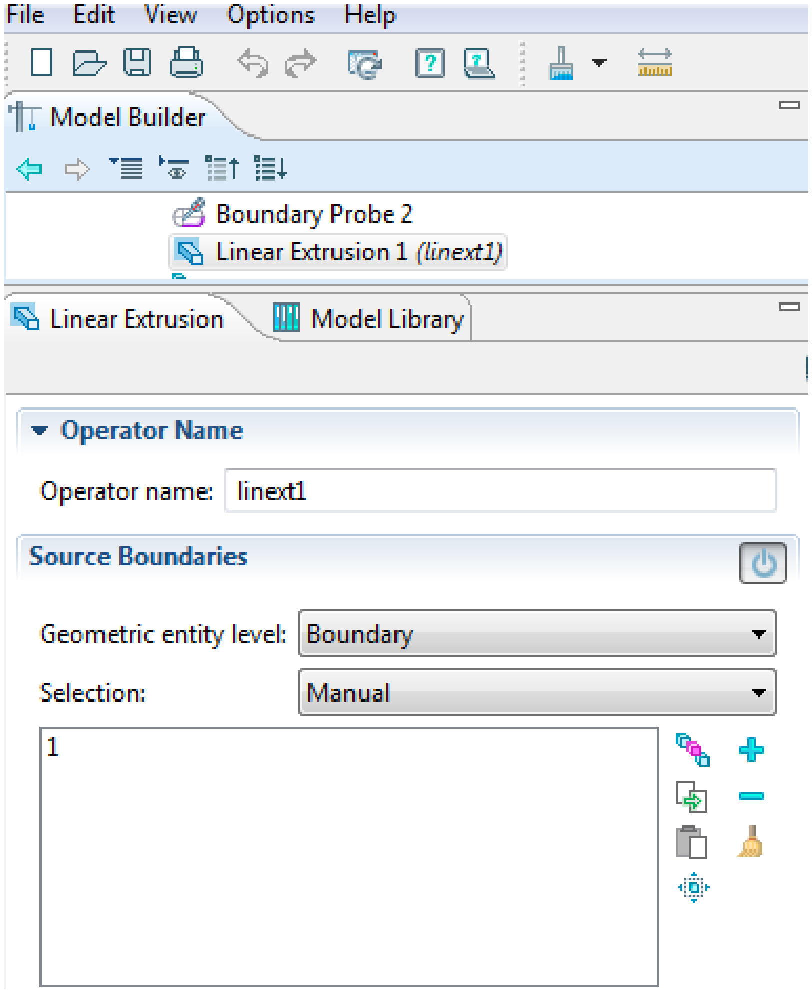
The pressure u on the east boundary is one less than on the west boundary. The pressure gradients (ux) are the same.



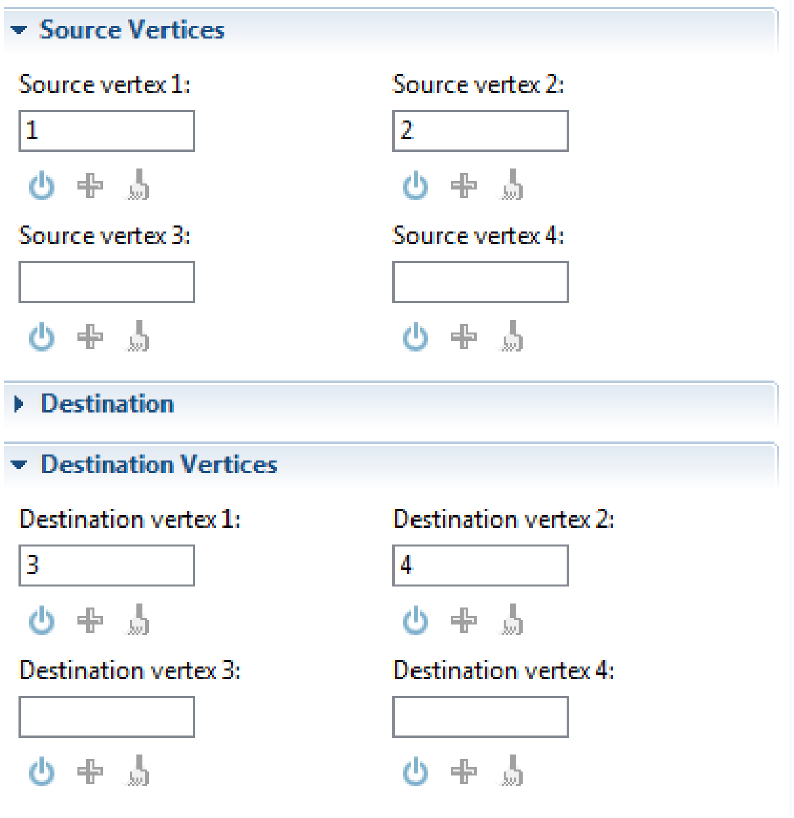
Define linear extrusion



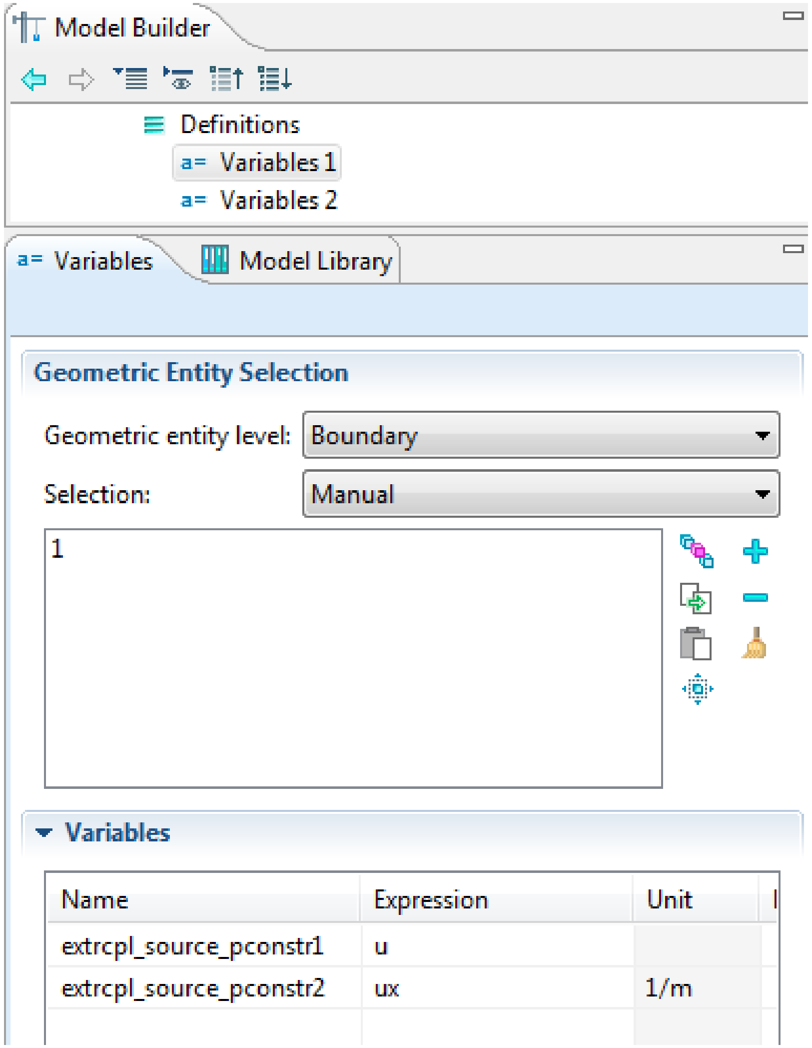
Choose linear extrusion



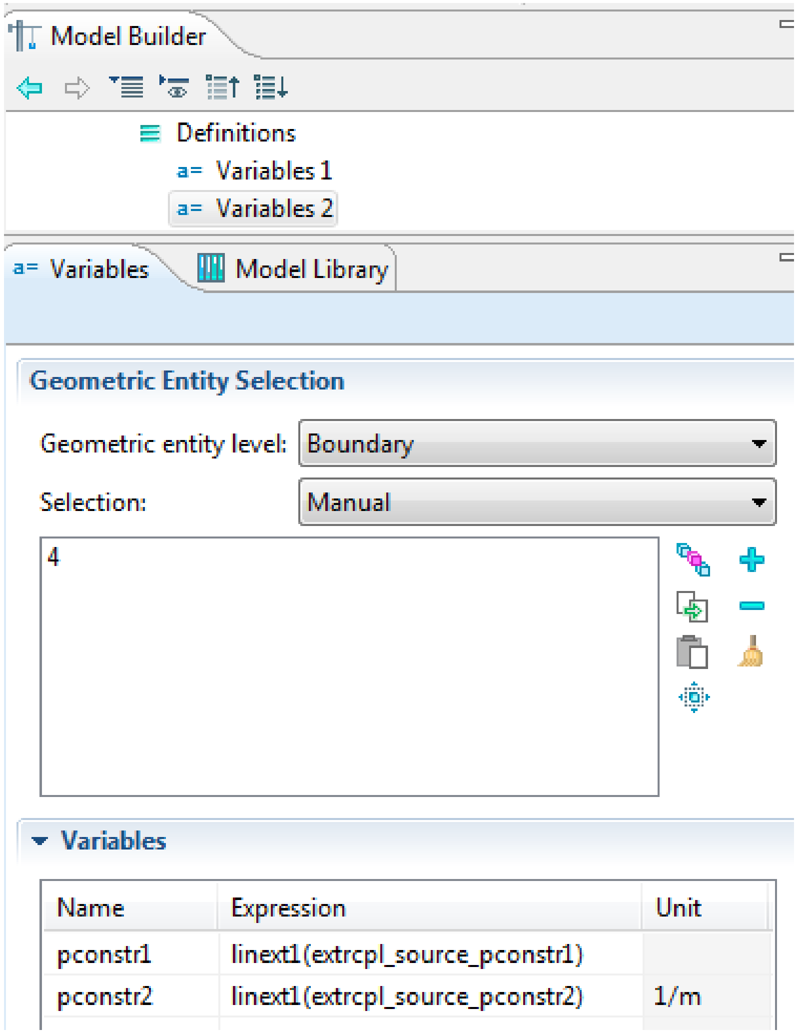
Scroll down to connect the right vertices



Define Variables 1 on the source boundary (1)



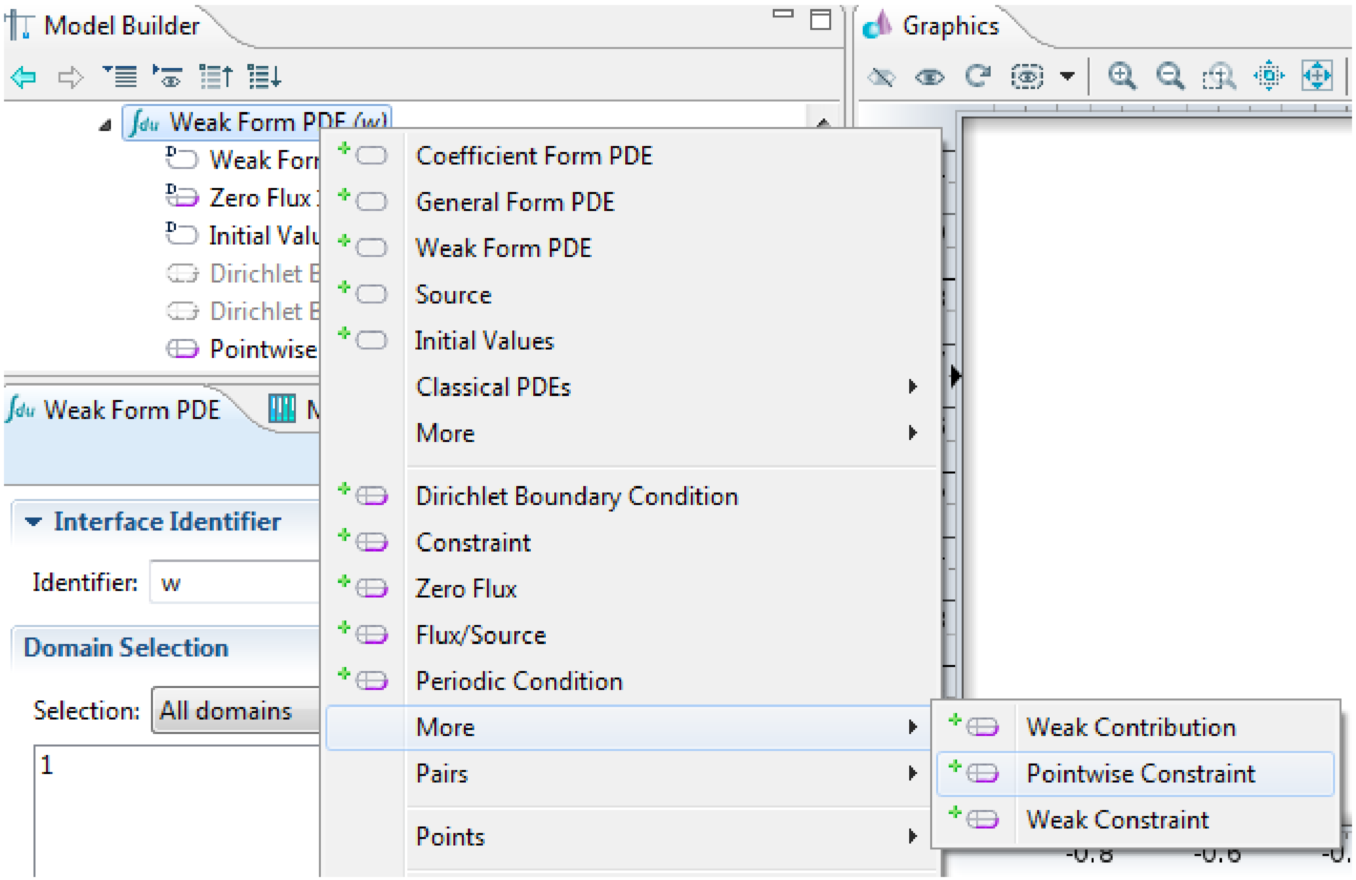
Define Variables 2 on the target boundary (4)



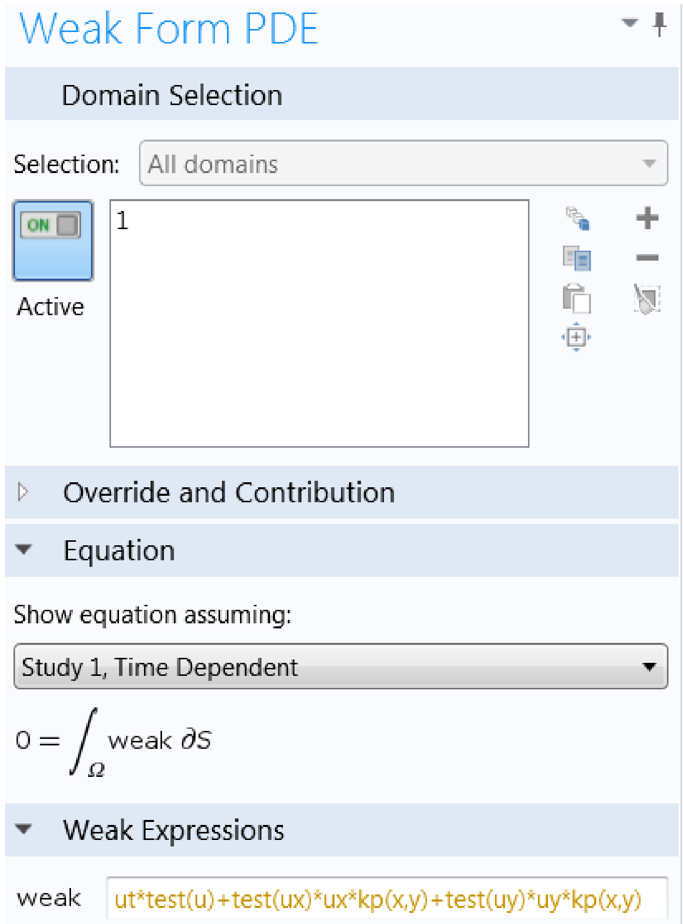
Linear Extrusion

- A Linear Extrusion coupling operator () maps an expression defined on a source to an expression that can be evaluated in the destination. Use this to define a linear mapping of this kind. Linear extrusion can be used when the correspondence between evaluation points in the source and destination is linear and in some nonlinear cases. Otherwise, use a general extrusion coupling. The Linear Extrusion operator defines a linear extrusion that maps between geometric parts of the same dimension

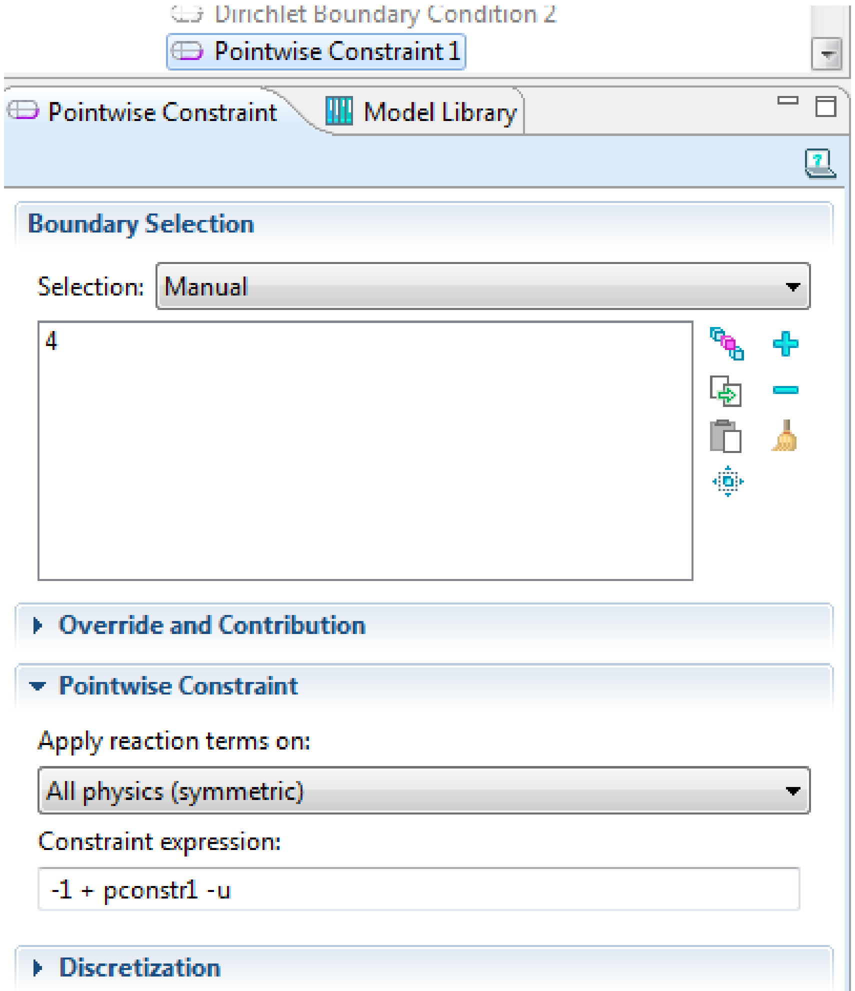
Right click on weak form of PDE and choose Pointwise Constraint



Right click on weak form of PDE and choose Pointwise Constraint

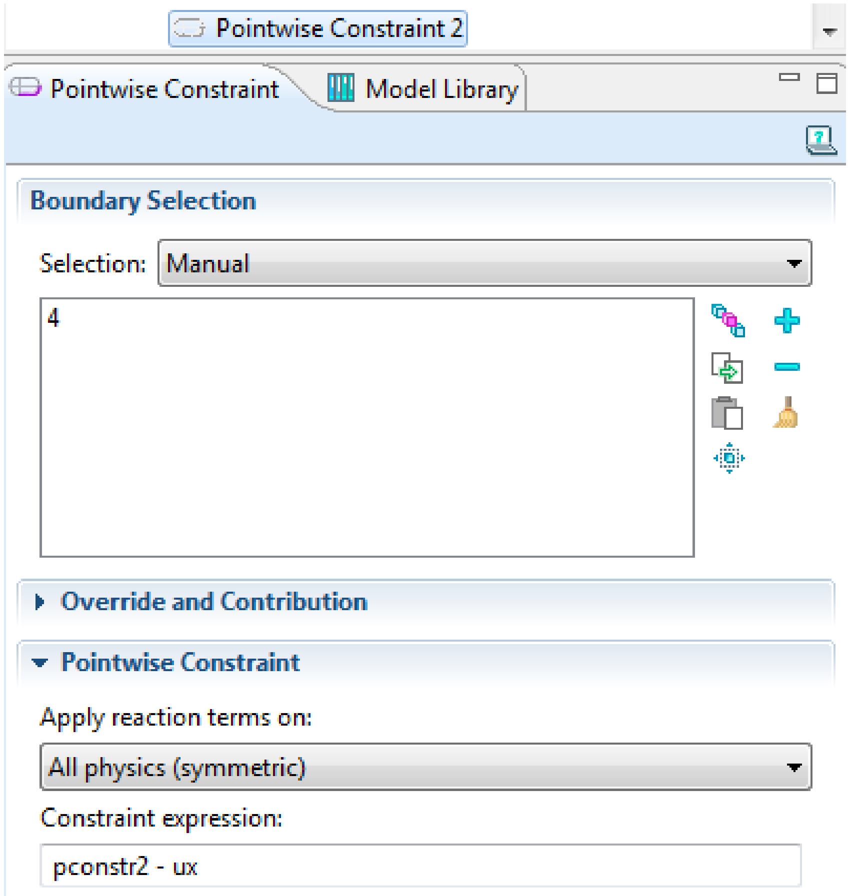


Choose target boundary (4) and give the constraint expression



-1+pconstraint1+u, means that at the source boundary, the value of *u* is one more than at the target boundary

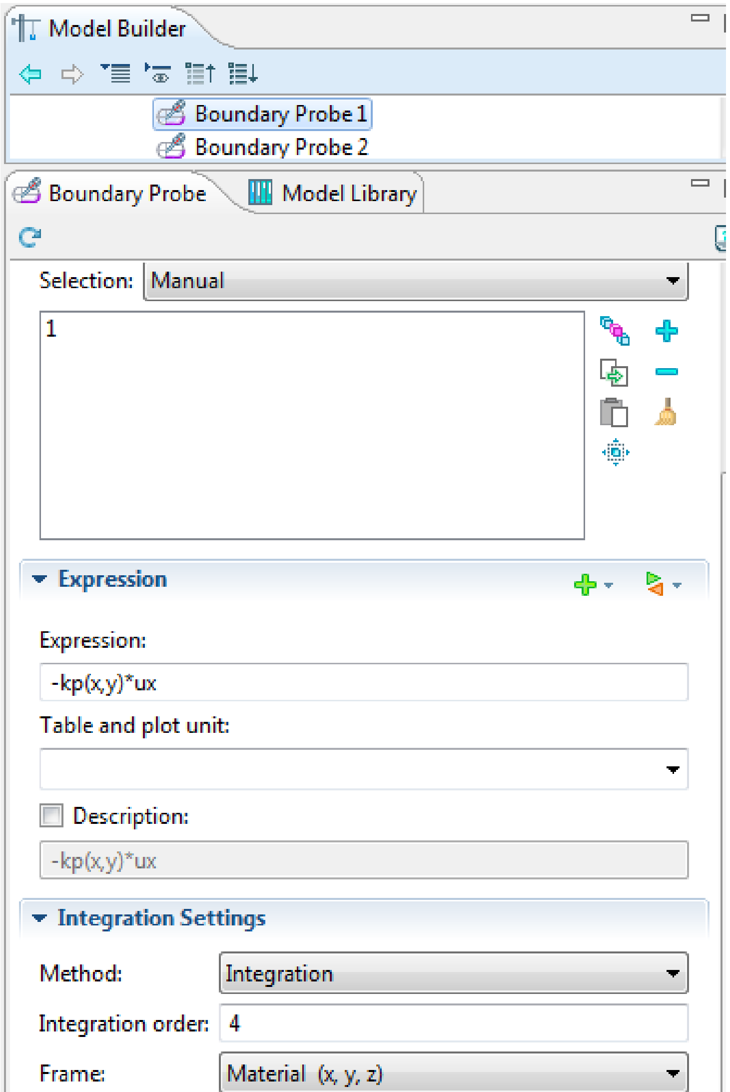
Repeat: Choose target boundary (4) and give the constraint expression



=ux+pconstraint 2, means that at the source boundary, the value of *ux* is the same as at the target boundary

This concludes the definition of the semi-periodic boundary conditions

Boundary probe



The average velocity on the east and west boundary (viscosity =1, unit square) is the average permeablity

Some observations

- The average permeability, for a homogeneous statistical field, does not depend on the boundary condition (Dirichlet, Neuman or periodic) if a separation of scale is possible (see A. Bourgeat and A. Piatnitski. Approximations of effective coefficients in stochastic homogenization. Annales de l'Institut Henri Poincaré/Probabilités et statistiques, 40(2):153165, 2004).