Notes on Spatial and Temporal Discretization
(when working with HYDRUS)

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1. Temporal Discretization

Four different time discretizations are used in HYDRUS: (1) time discretizations associated with the numerical solution, (2) time discretizations associated with the implementation of boundary conditions, (3) time discretizations which provide printed output of the simulation results (e.g., nodal values of dependent variables, water, solute mass balance components, and other information about the flow regime), and (4) time discretizations associated with data defining the objective function in the inverse mode of HYDRUS (e.g., measured water contents, pressure heads, concentrations, and/or fluxes).

Discretizations 2, 3, and 4 are mutually independent; they generally involve variable time steps as described in the input data file. Discretization 1 starts with a prescribed initial time increment, $\Delta t_{\text{init}}$. The time increment, $\Delta t$, is automatically adjusted at each time level according to the following rules:

a. Discretization 1 must coincide with time values resulting from time discretizations 2, 3, and 4.

b. Time increments cannot become less than a preselected minimum time step, $\Delta t_{\text{min}}$, nor exceed a maximum time step, $\Delta t_{\text{max}}$ (i.e., $\Delta t_{\text{min}} \leq \Delta t \leq \Delta t_{\text{max}}$).

c. If, during a particular time step, the number of iterations necessary to reach convergence is $\leq 3$ ($I_{\text{crit}}$), the time increment for the next time step is increased by multiplying $\Delta t$ by a predetermined constant $>1$ ($k_1$, usually between 1.1 and 1.5). If the number of iterations is $\geq 7$ ($I_{\text{crit}}$), $\Delta t$ for the next time level is multiplied by a constant $<1$ ($k_2$, usually between 0.3 and 0.9).

d. If, during a particular time step, the number of iterations at any time level becomes greater than a prescribed maximum ($I_{\text{crit}}$, usually between 10 and 50), the iterative process for that time level is terminated. The time step is subsequently reset to $\Delta t/3$, and the iterative process restarted.

Parameters $\Delta t_{\text{init}}$, $\Delta t_{\text{min}}$, $\Delta t_{\text{max}}$, $I_{\text{crit}}$, $I_{\text{min}}$, $I_{\text{max}}$, $k_1$, and $k_2$ are be specified by a user at the input. The recommended values for these parameters are as follows:
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Recommended Value</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta t_{\text{init}}$</td>
<td>1 s (15 minutes)</td>
<td>Initial time increment, $\Delta t$ [T]. The recommended value for the initial time step depends on the type of simulation and boundary conditions used. When simulating a process that starts with a large initial pressure head or concentration gradient at the boundary (e.g., ponded infiltration or a sudden change of boundary concentration), use a small value of the initial time step (e.g., 1 s). When simulating a long term process with variable boundary conditions (e.g., seasonal or multiyear simulation), start with a larger time step (e.g., 15 min). This is because this initial time step is used whenever time variable boundary conditions significantly change (e.g., the water flux changes by 25% or more). If needed (if there is no convergence for $\Delta t_{\text{init}}$), the program will still use a smaller time step than $\Delta t_{\text{init}}$, but starting with larger $\Delta t_{\text{init}}$ leads to more efficient calculations. In general smaller initial time steps must be used for soil with more nonlinear soil hydraulic properties (e.g., course textured soils) and larger initial time steps can be used for soil with less nonlinear soil hydraulic properties (e.g., loam).</td>
</tr>
<tr>
<td>$\Delta t_{\text{min}}$</td>
<td>1 s</td>
<td>Minimum permitted value of the time increment, $\Delta t_{\text{min}}$ [T]. The minimum time step must be smaller than a) the initial time step, b) interval between print times, and c) interval between time-variable boundary condition records. Always specify a small minimum allowed time step, on the order of 1 s. This value may never be used, but it provides the code with flexibility when it may be needed, e.g., when there is a sudden change in boundary fluxes and HYDRUS may not converge with larger time steps.</td>
</tr>
<tr>
<td>$\Delta t_{\text{max}}$</td>
<td>Large</td>
<td>Maximum permitted value of the time increment, $\Delta t_{\text{max}}$ [T]. This is a relatively unimportant parameter and a large value may be specified. Since HYDRUS automatically selects its optimal time step, there is usually no need to constrain that. The only time when there is a need to constrain the time step is likely for cases when HYDRUS is asked to generate internally intra-daily variations in temperature, or in evaporation and transpiration fluxes. Then there is a need to have time step smaller (e.g., 1 h) so that these daily variations can be properly modeled.</td>
</tr>
<tr>
<td>$I_{\text{crit}}$</td>
<td>10</td>
<td>Maximum number of iterations allowed during any time step while solving the nonlinear Richards equation using a modified Picard method. The recommended and default value is 10. It is usually not helpful to use a larger value than 10. If HYDRUS does not converge in 10 iterations, then there is a relatively small probability that it will do so during more iteration. Even if it does, it is much more efficient to reduce the time step and attempt to find the solution with a smaller time step, which is done automatically by the program when $I_{\text{crit}}$ is reached.</td>
</tr>
<tr>
<td>$I_{\text{min}}$</td>
<td>3</td>
<td>Optimal value in most cases.</td>
</tr>
<tr>
<td>$I_{\text{max}}$</td>
<td>7</td>
<td>Optimal value in most cases.</td>
</tr>
<tr>
<td>$k_1$</td>
<td>1.3</td>
<td>Optimal value in most cases. Only when there is a saturated zone in the profile, e.g., a perched water layer, the numerical solution may be more stable with smaller $k_1$ (e.g., 1.1).</td>
</tr>
<tr>
<td>$k_2$</td>
<td>0.7</td>
<td>Optimal value in most cases.</td>
</tr>
</tbody>
</table>
2. Spatial Discretization

2.1. FE-Mesh in HYDRUS-1D

The finite element mesh is constructed by dividing the soil profile into linear elements whose sizes are defined by the $z$-coordinates of the nodes that form the element corners.

2.2. FE-Mesh in HYDRUS (2D/3D)

The finite element mesh is constructed by dividing the flow region for two-dimensional problems into quadrilateral and/or triangular elements or for three-dimensional problems into tetrahedral, hexahedral and/or triangular prismatic elements whose shapes are defined by the coordinates of the nodes that form the element corners. The program automatically subdivides the quadrilaterals into triangles (or hexahedrals and triangular prisms into tetrahedrals), which are then treated as subelements.

2.3. Common Rules

In general, the finer the FE-mesh size is, the more precise the results will be. On the other hand, the number of calculation steps increases, as additional equations must be solved for every further FE node. This affects the computing time considerably. A mesh size that is too fine slows down the calculation without improving the quality of the analysis significantly. On the other hand, a coarse mesh may not capture the boundary conditions in a satisfying way and the numerical solution may not converge.

Finite element dimensions must be adjusted to a particular problem. They should be made relatively small at locations where large hydraulic gradients are expected. Such a region is usually located close to the soil surface where highly variable meteorological factors can cause rapid changes in the soil water content and corresponding pressure heads. Similarly, regions with sharp gradients can be located in the vicinity of the internal sources or sinks. Hence, we recommend normally using relatively small elements at and near the soil surface. The size of elements can gradually increase with depth to reflect the generally much slower changes in pressure heads at deeper depths. We also recommend using elements having approximately equal sizes to decrease numerical errors. The ratio of the sizes of two neighboring elements is not recommended to exceed about 1.5.

The required size of finite elements close to the soil surface depends very much on how boundary conditions are specified. When boundary conditions are specified for daily, or shorter, time intervals, usually resulting in short-duration fluxes of a large magnitude, spatial discretization needs to be finer (on the order of cm) than when boundary conditions are specified for longer time intervals (e.g., weekly or monthly).

The element dimensions should also depend upon the soil hydraulic properties. For example, coarse-textured soils having relatively high $n$- and $\alpha$-values generally require a finer discretization than fine-textured soils. That is because their soil hydraulic functions are more nonlinear and thus the numerical solution may be less stable. To demonstrate this issue, we have carried out
simulations of ponded infiltrations into sand and clay soil profiles (see Figure 1). Notice that the pressure head front for a sandy profile is very sharp and the entire front is only about 5 cm thick. To be able to describe this front using our numerical model, we need several FE nodes at the front, implying that our spatial discretization must be on the order of 1 cm or less. On the other hand, the pressure head (and correspondingly water content) front for a clay profile is relatively smooth and consequently our spatial discretization can be much coarser.

Figure 1. Pressure head profiles for ponded infiltration into sand and clay soil profiles.

2.4. HYDRUS (2D/3D) Rules

In higher dimensions, it is often recommended that in order to obtain smooth solutions, FE elements should have approximately all sides equal. This recommendation is not valid for most applications involving fluxes in the vadose zone. Since in the vadose zone vertical fluxes usually dominate over horizontal fluxes, the spatial discretization must be much finer in the vertical direction than in the horizontal direction. In general, the spatial discretization should reflect the expected gradients in the transport domain; it should be fine in the direction of large gradients and can be coarser in the direction of small gradients.

HYDRUS offers several parameters and tools to adjust the spatial discretization to expected flow and transport conditions. The four most important parameters and tools are the Targeted FE Size, the Smoothing Factor, Mesh Stretching, and the FE-Mesh Refinement. The first three parameters can be specified in the FE Mesh Parameters dialog window, which can be displayed by clicking on the menu command “Edit->FE-Mesh->FE-Mesh Parameters” or the FE-Mesh Parameters command (FE-Mesh Parameters...) at the Tools Sidebar when the FE-Mesh View is displayed.

HYDRUS uses two different FE-Mesh generation modules. It uses the MeshGen module to generate FE meshes for two-dimensional domains and for the Base Surface of three-dimensional layered domains. It then uses the Genex module to generate FE meshes for three-dimensional general domains (note that three-dimensional general domains are available only in the Professional Level of HYDRUS to be released in spring 2010). These are relatively different approaches to generating FE meshes and thus the use of the above discussed parameters and tools is sometimes also different. In the text below we will attempt to emphasize these differences.
2.4.1. Targeted FE Size

The Targeted FE Size (see Figure 2) defines the global FE mesh size, i.e., the size of finite elements that the FE-Mesh generator will try to reach throughout the transport domain. FE-Mesh can be made finer or coarser in different parts of the transport domain by defining FE-Mesh Refinements (see discussion below) for these parts of the domain.

![Figure 2. The FE-Mesh Parameters dialog window with the Main Tab displayed.](image)

Note that the Targeted FE Size that is suggested by HYDRUS (when the check box Automatic is on) is related only to the size of the transport domain, and is a certain fraction (e.g., 1/60) of the diameter of the transport domain. The purpose of this number is to suggest such size of finite elements, so that the number of elements is reasonable. The Automatic Targeted FE Size is not adjusted to any other factors involved in a particular project, such as nonlinearity of soil hydraulic properties, how the boundary conditions are defined, heterogeneity of the soil profile, and so on. Users need to adjust the Targeted FE Size for their particular problems themselves and then adjust the FE-mesh where needed using FE-Mesh Refinements as needed.

Note that the Targeted FE Size is used by GENEX in all three dimensions and by MeshGen in two dimensions (for the Base Surface of Layered Three-Dimensional domains). Distances between layers in Layered Three-Dimensional domains is defined differently (see below).
2.4.2. Smoothing Factor

The Smoothing Factor (see Figure 3) is the ratio of the maximum and minimum height of a finite element triangle. The Smoothing Factor is used only in for FE-meshes generated using MeshGen, i.e., for 2D and 3D-Layered domains, but not for FE-meshes generated using Genex, i.e., for 3D-General domains. For a triangle with equal sizes this factor is equal to 1 (which is theoretically not achievable for finite element meshes). The Smoothing Factor can be decreased to a value of about 1.1 when a highly smooth finite element mesh is required and, vice-versa, can be increased when a course mesh can be tolerated. The Smoothing Factor significantly affects the final number of elements, with the number of elements decreasing dramatically for larger values of the smoothing factor (e.g., 3). We recommend keeping the Smoothing Factor at its default value (i.e., 1.3) for relatively small transport domains (e.g., simulations of irrigation details), and increase its value to about 2-3 for larger transport domains (e.g., soil transects, field scale simulations) (see Figure 4).

![Figure 3](image-url)

Figure 3. The FE-Mesh Parameters dialog window with the MeshGen-Options Tab displayed.

![Figure 4](image-url)

Figure 4. Triangles with a smoothing factor equal to 1 (left) and 3 (right).
2.4.3. Stretching

Stretching of the finite element mesh (i.e., the degree of mesh anisotropy in a certain direction) is defined using the Stretching Factor and the Stretching Direction (see Figure 5). The finite elements are made larger in the particular Stretching Direction if the Stretching Factor is larger than one, and smaller if it is less that one. The result of this transformation is a mesh deformed in the given direction, which can be desirable for problems that, for example, require different spatial steps (mesh sizes) in the X, Y, and Z directions. As discussed above, in the vadose zone vertical fluxes usually dominate over horizontal fluxes, and thus the spatial discretization must be much finer in the vertical direction than in the horizontal direction. If vertical fluxes are expected to be many times larger (e.g., 10-100 times) in the vertical direction than in the horizontal direction, the Stretching Factor can also be very large (e.g., 10-100) (see Figure 6).

![Figure 5. The FE-Mesh Parameters dialog window with the Stretching Tab displayed.](image)

![Figure 6. Example of mesh stretching using a stretching factor of 3 in the y-direction.](image)
2.4.4. FE-Mesh Refinement

If no FE-Mesh Refinements have been defined, the FE mesh is generated with the preset Targeted FE size. The global FE mesh settings are described in chapter 2.4.1.

The mesh configuration can be affected by FE-Mesh Refinements that are set for selected parts of the computational domain. Use this option to refine the mesh where needed, such as at parts of the computational domains where large pressure head and/or concentration gradients are expected. Large pressure head and/or concentration gradients usually occur close to the soil surface (due to variable atmospheric fluxes), close to internal sinks/sources (drains, drippers, wells), or close to interfaces between different soil layers with significantly different soil hydraulic properties.

Using FE-mesh refinements one may try to find an appropriate compromise between results accuracy and computational time. Basically, there are four types of FE mesh refinements:

- Refinement around a node
- Refinement on a line
- Refinement on a surface
- Refinement on a solid (used only with Genex)

a) FE-Mesh Refinements in the MeshGen Module

Figure 7 shows New FE-Mesh Refinement dialog windows that are used with the MeshGen module for four different types of refinements. FE-Mesh Refinements can be applied to a Point, a Line, and a Surface.

When the FE-Mesh Refinement is assigned to a Point (Figure 7 top left), users only need to define the finite element size that is to be used at a given point. This FE-size will be used around a given point, while sizes of neighboring FE will be gradually increased until the Targeted FE Size is reached further away in the computational domain. Notice that the dialog window also displays the Global Targeted FE Size. The same FE-Mesh Refinement, i.e., the same refined FE size, can be assigned to multiple Points in the transport domain.

There are two ways how the FE-Mesh Refinement can be assigned to a Line (Figure 7 top right and bottom left). Users can either specify the FE-Size (Line – FE-Size; Figure 7 top right) or the Number of Points (Line – Number of Points; Figure 7 bottom left) to be used on the entire line. Similarly as for points, the FE-Size (either given directly or calculated from the number of points) will be used on the Line, while sizes of FE away from the Line will gradually increased until the Targeted FE Size is reached further away in the computational domain. Again, the same FE-Mesh Line Refinement, i.e., the same refined FE size, can be assigned to multiple Lines in the computational domain.

The FE-Mesh Refinement can also be assigned to a selected Surface (Figure 7 bottom right). In this case, users need to define FE-Size for a selected Surface. Note that this option is useful only
when multiple **Surfaces** are used in the computational domain. The refined FE-Size is then used on the entire surface, including boundaries with other **Surfaces**, and the **Targeted FE Size** is reached only further away in the other **Surfaces** of the computational domain.

The **Point** or **Surface** with an assigned **FE-Mesh Refinement** are indicated using the following marks: □ and □, respectively.

![FE-Mesh Refinement dialog windows](image)

Figure 7. The **FE-Mesh Refinement** dialog windows for the **MeshGen** module with four different types of refinements (applied to a **Point**, a **Line** with a given FE-size or the number of Points, and to a **Surface**).
b) FE-Mesh Refinements in the Genex Module

While the MeshGen module discretizes the computational domain into unstructured FE-mesh using triangles (in 2D) and tetrahedrals (in 3D), the Genex module uses primarily quadrilateral (in 2D) and hexahedral (in 3D) finite elements. Genex uses triangles only in parts of the domain where needed, e.g., when it refines the grid. Although quadrilateral or hexahedral elements may be generated by Genex, the computational module subdivides these elements into triangles or tetrahedrals, respectively. While the transition between domains with refined FE-mesh and domains with global mesh size in MeshGen is relatively smooth and gradual (see Figure 7), in Genex the extent of this transition zone is defined exactly by users (see Figures below). Similarly as MeshGen, the same FE-Mesh Line Refinements can be assigned to multiple Points, Lines, Surfaces, and Solids in the computational domain.

There are two ways how the FE-Mesh Refinement can be assigned to a Point (Figure 8). Users can use either Circular or Rectangular refinement. For a Circular Refinement around a point, a radial refinement area is defined around a node in all directions. Users need to specify the Radius of the refinement area, the Inner Targeted FE-Size (i.e., a FE-size immediately around a point), and the Outer Targeted FE-Size (i.e., a FE-size at the outer end of the radial refinement area). The Outer Targeted FE-Size should be equal or slightly smaller than the Global Targeted FE-Size. When generating the FE mesh, the mesh refinement is carried out gradually towards the center because the FE length at the periphery of the refinement area is usually identical with the global mesh width. For larger differences between the inner and outer FE length, it is recommended to set the radius not too small in order to avoid acute-angled triangular finite elements in the refinement area. For a Rectangular Refinement, a rectangular refinement area is defined around a node in all directions. Users need to specify the Side Length of the refinement area and the Inner Targeted FE-Size (i.e., a FE-size immediately around a point).

Figure 8. Circular (left) and rectangular (right) refinements around a node.

FE-Mesh Refinements assigned to a Line are handled in Genex similarly as in MeshGen. One can again define either the size (spacing; Line through FE-Length) or the number (a specific number of equidistant sub-divisions; Line through Division) of finite elements along a line. In the former case one needs to define the Target FE Length, in the latter case the Number of
**Division FE Nodes.** However, while in **MeshGen** there was a gradual increase in sizes of finite elements away from the **Line**, in **Genex** the refinement affects only one row of finite elements (Figure 9).

![Figure 9](image1.png)

Figure 9, Refinement on a line (by defining either the size or the number of finite elements along a line).

It is also possible to define **Fe-Mesh Refinements** for **Surfaces** or **Solids** (Figure 10). In both cases, users need to specify the **Targeted FE-Size**, which will be set as target size of the finite elements for the entire surface or solid.

![Figure 10](image2.png)

Figure 10. Refinements on a surface (left) or solid (right).
Figure 11. The FE-Mesh Refinement dialog window for the Genex module with six different types of refinements (applied to a Circular or a Rectangular Point, a Line with a given FE-size or a number of points, to a Surface, and to a Solid).
2.4.5. Vertical Discretization of 3D Layered Domains

3D-Layered Domains (Solids) are formed by a Base Surface (discretized into finite elements using the MeshGen module) and one or multiple Thickness Vectors. A Solid, i.e., its base surface and thickness vectors, is defined and can be edited in the Edit Solid dialog window that has four tabs: General (Figure 12), Sub-Layers, Thickness Profiles, and FE-Mesh. The General Tab provides information, which Base Surface and which Thickness Vectors define the solid. Vertical discretization when the Base Surface is in the horizontal plane or horizontal discretization when the Base Surface is in the vertical plane is then defined in the other three tabs (i.e., Sub-Layers, Thickness Profiles, and FE-Mesh).

The Sub-Layers Tab (Figure 13) informs whether the solid is divided into one or more Sub-Layers. Layers are other objects that can be used to subdivide a single solid. These layers can be used, for example, to keep constant thicknesses of selected horizons or constant discretization close to the soil surface (to get good estimates of evaporation) across the entire transport domain (solid). Sub-Layers are defined on a single Thickness Vector, the so called Master Thickness Vector.

It is possible in the Edit Solid dialog to define number of Sub-Layers and their Thicknesses. A Solid has always one Master Thickness Vector, which is one of Thickness Vectors of a Solid, that has a special meaning as described below.

A thickness of a Sub-Layer is calculated as follows:

- Thicknesses of Sub-Layers given in the Table are calculated on the Master Thickness Vector.
The sum of **Thicknesses of all Sub-Layers** should be equal to the length of the **Master Thickness Vector**. If it is not so, a program will issue a warning and recalculate **Thicknesses of Sub-Layers** automatically.

A **Solid** can have more **Thickness Vectors** of different lengths so that specified **Thicknesses of Sub-Layers** can not be maintained. The program then does the following:

For **Sub-Layers** with the **Constant Thickness Type**, the specified thickness is maintained at all **Thickness Vectors**, i.e., over the entire computational domain. For **Sub-Layers** with the **Variable Thickness Type**, their thicknesses are linearly increased or decreased so that the sum of **Thicknesses of all Sub-Layers** corresponds with the length of a particular **Thickness Vector**.

Figure 13. The **Edit Solid** dialog window with the **Sub-Layers Tab** displayed.

In the preceding paragraph we have described how to define **Thicknesses of Sub-Layers** on the **Master Thickness Vector** using a table. This table represents the so called **Master (Default) Profile**, i.e., a particular distribution of thicknesses. If one wants to define precisely the division of thicknesses also on other vectors than the **Master Thickness Vector**, then it is necessary to create additional **Thickness Profiles** and use them on corresponding **Thickness Vectors**. One **Thickness Profile (Default Profile)** is created by the code automatically. Figure 14 shows a dialog (the **Thickness Profiles Tab** of the **Edit Solid** dialog) for the creation of additional **Thickness Profiles**. There is always a **Default Profile**, which corresponds to the table described in Figure 13 above. One can create new profiles, change their thicknesses or delete them. One can simultaneously also see a list of **Thickness Vectors** where the selected **Thickness Profile** is used.

These additional **Thickness Profiles** must be subdivided into the same number of **Sub-Layers** as the **Default Profile** and these **Sub-Layers** can have either constant or variable thickness (T) across the transport domain. Thicknesses and the mode (constant or variable) of particular layers...
are specified in a table. Thickness Sum (TT) is then calculated by adding thicknesses of particular layers. At least one layer thickness must be variable. The finite element discretization then follows these layers.

Finally, the FE-Mesh Tab (Fig. 15) specifies how many horizontal FE-Layers are used to discretize the solid. When only one Sub-Layers (Figure 13) exists then users can specify relative finite element spacing (spacing of vertical discretization layers) on the vertical side (FE-Mesh Layer Spacing) using the RS1 (relative size at the top) and RS2 (relative size at the bottom) factors below Generate Mesh Layer Spacing. The element sizes are then proportionally distributed. The preview part of the dialog window shows the main terms used on each Tab. When multiple Sub-Layers (Figure 13) exist then users can specify relative sizes of elements for each layer (FE-Mesh Density in Layers).
Figure 15. The **Edit Solid** dialog window with the **FE-Mesh Tab** displayed for a single (top) and multiple layers (bottom).
2.4.6. FE-Mesh Generation

To start the FE mesh generation, select the **Generate FE-Mesh** command (Generate FE-Mesh) in the **Calculation** menu or at the Tools Sidebar.

It is recommended, to check the generated FE-mesh before the calculation is started. In this way, you can find out whether efficiently refined mesh has been created or if refinement areas are still required. It is also possible that areas that are of minor interest for the results evaluation are covered by a coarser FE-mesh. You can define, for example, a **FE-Mesh Refinement** with a **Targeted FE-Size** larger than the defined target size. This speeds up both analysis and results output.

If the FE mesh generation has been successful, select the **FE-Mesh Statistic** command (FE-Mesh Statistics...) in the **Calculation** menu or at the Tools Sidebar to open a dialog box with information about the generated FE mesh.

![FE-Mesh Information dialog window](Figure 16. The FE-Mesh Information dialog window.

The statistics show the types and numbers of the generated finite elements, which is helpful in order to select the appropriate matrix solver method and to judge the approximate calculation time.

To delete the mesh select the **Delete FE-Mesh** command (Delete FE-Mesh) in the **Calculation** menu or at the Tools Sidebar. When you use this function, all results that may be available will be deleted, too.