STUDENT SUMMER INTERNSHIP TECHNICAL REPORT

Investigation of the Workflow to Construct an Integrated Hydrology Model for Basin 6 of the Waste Isolation Pilot Plant (WIPP)

DOE-FIU SCIENCE & TECHNOLOGY WORKFORCE DEVELOPMENT PROGRAM

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EXECUTIVE SUMMARY

This research work has been supported by the DOE-FIU Science & Technology Workforce Development Initiative, an innovative program developed by the U.S. Department of Energy's Office of Environmental Management (DOE-EM) and Florida International University's Applied Research Center (FIU-ARC). During the spring of 2022, a DOE Fellow intern, Aubrey Litzinger, spent ten weeks doing a summer internship at Los Alamos National Laboratory under the supervision and guidance of Dr. David Moulton and Dr. Yu Zhang. The intern's project was initiated on June 6, 2022, and continued through August 12, 2022, and was focused on learning the workflow for development and visualization of an integrated hydrology model using open-source tools such as TINerator, Advanced Terrestrial Simulator (ATS), VisIt, and ParaView. The goal was to develop and visualize an integrated surface/subsurface hydrology model for a small pilot study area (~3.7 km^2) within Basin 6, that lies just west of the Waste Isolation Pilot Plant (WIPP). Working with a small sub-basin allowed for faster generation of results and made it easier to resolve errors before the workflow is to be performed on the entire area of interest. This enabled the DOE Fellow to obtain modeling experience as well as an understanding of model run time at high grid resolutions.

The WIPP which is located in Carlsbad, New Mexico, and is the only existing deep geologic long-lived radioactive waste repository in the U.S. It was constructed within a geologic salt layer over 2,000 feet below the ground to isolate low-level, transuranic, radioactive waste. A significant concern of DOE-EM scientists is the long-term performance and vulnerability of the karst topography surrounding the WIPP and, more specifically, how surface features such as sinkholes, swallets, and karst valleys will influence the groundwater recharge which can potentially result in accelerated dissolution of the subsurface geological layers. It is therefore important to investigate and have a good understanding of the relationship between the groundwater recharge and seasonal monsoon precipitation events. To address these concerns, a detailed model is needed that can couple surface and groundwater processes. The Advanced Terrestrial Simulator (ATS), which is an open-source model capable of analyzing surface and groundwater flows, was selected for this purpose. ATS is an ecosystem-based, integrated, distributed hydrology simulator built upon the underlying multi-physics framework provided by Amanzi, the high-performance computing simulator. Amanzi was developed in the Advanced Simulation Capability for Environmental Management (ASCEM) program. The hydrological model development for this work focused on Basin 6 located within the Nash Draw Basin near the WIPP site. Nash Draw contains 30 internally drained sub-basins. The objective of the internship was to generate an integrated hydrology model for a sub-basin of Basin 6 using ATS after exploring the workflow using multiple scenarios based on a watershed at the Canadian Forces Base Borden in Ontario, Canada. This sub-basin contained two sinkholes, which are surface features of interest due to their capacity to increase subsurface infiltration. The methodology consisted of creating an unstructured mesh of the sub-basin using the Python module TINerator, and then generating an XML input file to control the ATS simulations. This input file specifies regions within the mesh, simulation times, equations, meteorological data, geological data, soil parameters, and other essential elements ATS needs to generate an integrated hydrological model. After ATS configures and simulates the model from the XML input file, the results can be visualized using the open-source software, VisIt, and

ParaView. The results of this internship will then be used to develop an integrated hydrology model for the entire region of Basin 6 at Florida International University's Applied Research Center.

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1. INTRODUCTION

Southern New Mexico contains the only deep geologic long-lived radioactive waste repository in operation in the U.S. This waste repository, known as the Waste Isolation Pilot Plant (WIPP), is located 2,150 feet underground in Carlsbad, New Mexico. The WIPP site permanently isolates low-level, transuranic, radioactive waste within a layer of salt known as the Salado Formation. Above the Salado Formation is the Rustler Formation, which has three fluid-bearing zones. Only two are located within the WIPP site, the Magenta and Culebra dolomite zone. Also located in the WIPP area is the Nash Draw Basin, which is an enclosed basin that contains 30 internally drained basins. Basin 6 of the thirty Nash Draw sub-basins has been the focus of this work. Figure 1 shows an aerial image of the WIPP site, the Nash Draw basin, and Basin 6 highlighted in red.
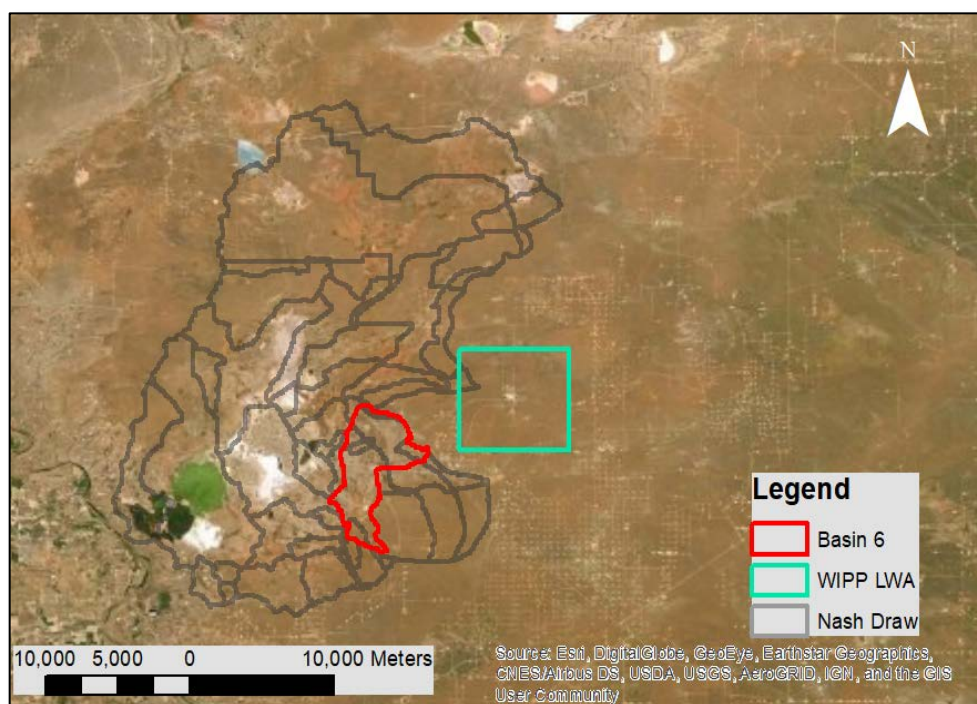
Figure 1. Aerial View of the Geographical Relationship Between Basin 6, The WIPP Site, and Nash Draw.

A significant concern of DOE-EM scientists is the long-term performance and vulnerability of the karst topography surrounding the WIPP and, more specifically, how surface features such as sinkholes, swallets, and karst valleys will influence the groundwater recharge and potentially result in accelerated dissolution of the subsurface geological layers. It is therefore important to investigate and have a good understanding of the relationship between the groundwater recharge and seasonal monsoon precipitation events in order to estimate the rate of propagation of the shallow dissolution front. To address this concern, there should be research on the regional water balance (Chaturvedi, 1993).

As the significant surface hydrological features are present at a very small scale (meters), a high-resolution hydrological model is needed to accurately represent hydrological flow variability across small scales. Therefore, a high-resolution (1-meter) digital elevation model was developed

of the site using a recently released United States Geological Survey (USGS) source data product (including a LiDAR point cloud dataset) derived from unmanned aerial vehicle (UAV)-based photogrammetry and used to develop a fully integrated surface/subsurface hydrological model using the open-source Advanced Terrestrial Simulator (ATS) to analyze surface and groundwater flows. ATS is an ecosystem-based, integrated, distributed hydrology simulator built upon the underlying multi-physics framework provided by Amanzi, the high-performance computing simulator. (Coon et al., 2016). The Department of Energy Office of Biological and Environmental Research (DOE BER) supported the development of ATS, which builds on Amanzi and naturally integrates with the Advanced Simulation and Capability for Environmental Management Program (ASCEM). ATS is used to solve coupled surface and subsurface hydrology problems, which may include surface energy balance, snow processes, freeze/thaw processes, dynamic vegetation, and reactive transport processes. ATS uses a process kernel tree, which is comprised of processes and couplers, to help the user represent the model configuration while providing a rigorous mechanism to capture the relationship of all variables, equations, and predefined fields used in the simulation.

The internship was focused on developing an understanding of the workflow, input requirements and tools required to create an ATS model and perform simulations based on various meteorological scenarios. This includes the generation of meshes from a DEM, addition of surface and subsurface features into a mesh, development of input files for the ATS simulation, execution of ATS simulations, and then the visualization and analysis of ATS output files. Before the internship, the development of meshes in the workflow was understood; therefore, the internship's main focus was the ATS modeling component. The work was documented through GitHub, in which Jupyter notebooks were used to create the mesh, and the ATS input files used to run the simulation were stored.

In order to practice the workflow of performing ATS simulations, the Borden watershed, a small well-studied watershed on the Canadian Forces Base Borden in Ontario, Canada, was used as a reference. The workflow referenced in the Borden watershed problem was used for two smaller sub-basins of Basin 6. The experience and skills gained during the internship will be used to develop an integrated surface/subsurface hydrology model for the entire Basin 6 region using a high-resolution DEM generated by UAV photogrammetry methods.

2. RESEARCH DESCRIPTION

The Borden watershed, located in Ontario, Canada, has been used to test multiple hydrology simulators. The Borden watershed was recently used to evaluate several popular integrated hydrology codes in a model intercomparison study published by Kollet (2017) [4]. The Borden watershed was used as benchmark data against ATS and other modeling programs in this study. Since the watershed is a relatively small and well-studied case, it was used as a reference case for the ATS workflow development.

For developing integrated hydrology models of the region near the WIPP site, the Borden watershed was used to develop components of the workflow and evaluate the ATS capability. Since the generation of meshes was previously understood before the internship, it is only briefly described below in the workflow.

2.1 Workflow for the ATS Model Development, Visualization and Analysis

The ATS workflow begins with collection and processing of input data. Next, a mesh is generated, followed by an ATS input file. Simulations are then performed using ATS, and the output data is visualized and analyzed. This workflow is seen in Figure 2.
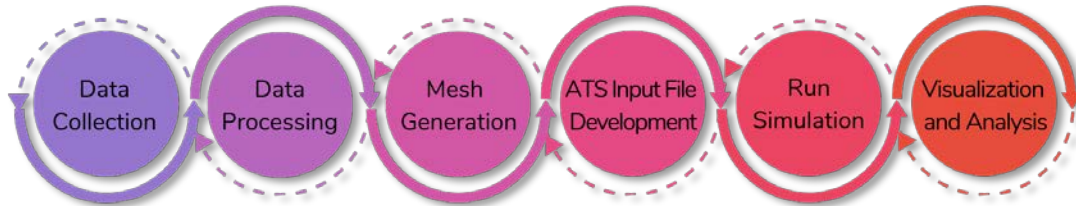
Figure 2. The workflow flows to the right (solid arrows), but issues may arise at any step and result in backtracking to the previous step or require iterations (dashed arrows).

A digital elevation map (DEM) was an essential element of the data collection and data processing. The DEM is used to generate the mesh, for which the python module, TINerator, is used. TINerator was developed by Los Alamos National Laboratory (LANL) and was the chosen python module to create the unstructured, triangulated meshes which were exported as ExodusII files. The ExodusII format allows for geometrical and geophysical information about the site to be encoded into the ATS input file (Livingston, 2020).

After the creation of the mesh, an ATS input file is generated. The input file is written in XML format and configures the set of coupled processes for the simulation at run time. This input file also defines all aspects of the hydrological model, such as meteorological data, geometric regions, the process kernel tree, and visualization output. The following significant sections of the input file were defined in this model:

1. The mesh in ExodusII format
2. The regions using the mesh as a reference point
3. The cycle driver that determines the run time
4. The process kernel tree (PK tree) which details each PK and multi-process coupler (MPC) used, such as:

       a. PKs:
           i. Richards PK
           ii. Overland flow PK
       b. MPCs:
           i. Coupled water
5. State and field evaluators that define variables relating to the area, such as:
       a. Water table level
       b. Surface ponded water depth
       c. Precipitation
       d. Surface temperature
       e. Surface overland conductivity
       f. Surface manning coefficient
6. Directions for the generation of visualization output files
7. Observations that allow for a more in-depth analysis of variables
8. Checkpoints for status on the simulation run

After the simulation is run using the ATS input file described above, visualization files generated during the run are imported into visualization software like ParaView or VisIt. ParaView was created by Kitware Inc. and Los Alamos National Laboratory and is an open-source, multi-platform data analysis and visualization application. VisIt is an open-source, interactive, scalable visualization, animation, and analysis tool developed by the Department of Energy (DOE) Advanced Simulation and Computing Initiative (ASCI).

2.2 Workflow of the Borden Watershed Model Development

2.2.1 Generating the Mesh and Sets for the Borden Watershed

Prior to the internship, the Fellow had a good understanding of the process for generation of an ExodusII mesh. This process was performed in Jupyter Lab using the python module, TINerator. A DEM obtained from the Kollet study was imported into Jupyter Lab, and a watershed delineation was performed. This is done by filling depressions of the DEM, resolving flats, and then performing flow accumulation. The flow network can then be extracted with an accumulation threshold, as all cells above that threshold are a part of the network. In TINerator, the D8 flow accumulation method was used to develop the raster to guide the refinement of the unstructured mesh around the streams.

The next part of generating an unstructured mesh was to create the surface mesh by using a triangulation function with TINerator. The minimum and maximum edge lengths of the triangles used in the mesh needed to be defined. The method used for the triangulation function was called "jigsaw," which was chosen due to its ability to create high-quality Delaunay triangulation on the surface. The scaling method also needs to be identified, in which a "Relative" method was chosen so that the edge lengths will be a percent of the DEM extent.

After the surface mesh was created for the Borden watershed, vertical layers were added to the mesh to create depth. The sets were then defined by TINerator with a naming convention that would allow them to be identified individually in the ATS input file later. The sets labeled were "top_face", "bottom_face", and "side_face". The "side_face" was the boundary of the mesh. The

layers were also numbered one through three, with one being the top layer and three being the bottom layer. Another set that was established marked the outlet of the watershed. This set was created by identifying two points on the boundary of the surface mesh, and using a TINerator function to collect the faces of the mesh along this boundary segment to create the "outlet" set. The sets, faces, and mesh were compiled together to be exported as the final ExodusII mesh. This mesh can be seen in Figure 3 with the three layers.
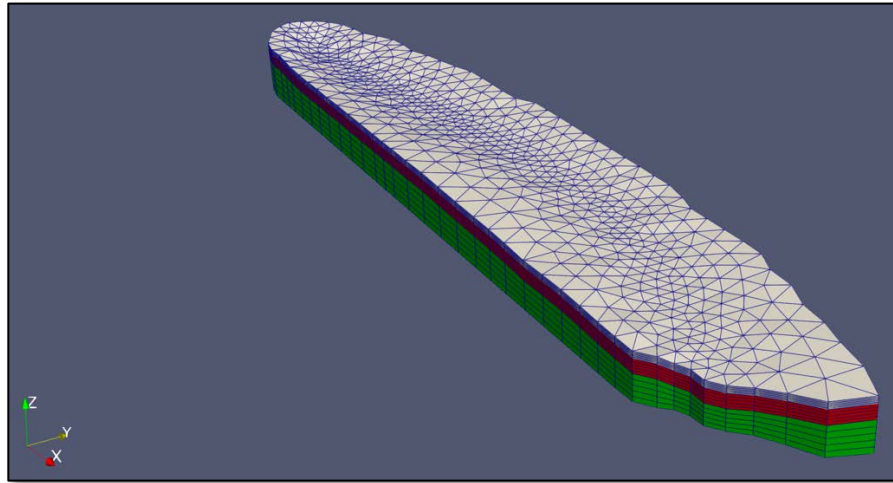
Figure 3. Mesh generated using TINerator with the three layers shown.

The mesh generated shows the smaller triangulation along the watershed line that was identified using TINerator. The mesh also shows the three layers, with white being the surface, red being the middle, and green being the bottom layer. These were labeled 1, 2, and 3, with 1 being the top and 3 being the bottom.
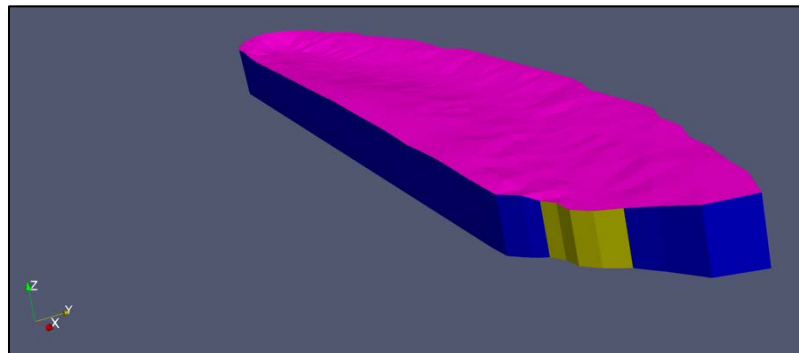
Figure 4. Sets generated and labeled using TINerator visualized in the model.

The sets labeled in TINerator can be visualized in the model. As seen in Figure 4, the sets that are being visualized are the top face, side face, bottom face, and outlet. These sets have reference numbers labeled in TINerator so that they can be referred to later in the ATS input file. The reference numbers for each set were:

- Boundary = 30 (Blue color)
- Outlet = 31 (Yellow color)
- Top face set = 32 (Pink color)

- Bottom face set = 33 (not visible)

2.2.2 Developing the ATS Input File for the Borden Watershed

For the development of the ATS input file, the Richards' equation was used for the subsurface and the diffusive wave model for the surface (overland flow), in which they were coupled by continuous pressure formulation. Mimetic finite differences (MFD) were also used to maintain accuracy when working on the unstructured meshes added to the input file. Multiple scenarios were created to understand how an ATS input file is developed fully, and input files for each scenario were formed for practice. These scenarios were established as a good practice tool, and then applied to the Borden watershed. The scenarios are seen in Figure 5.
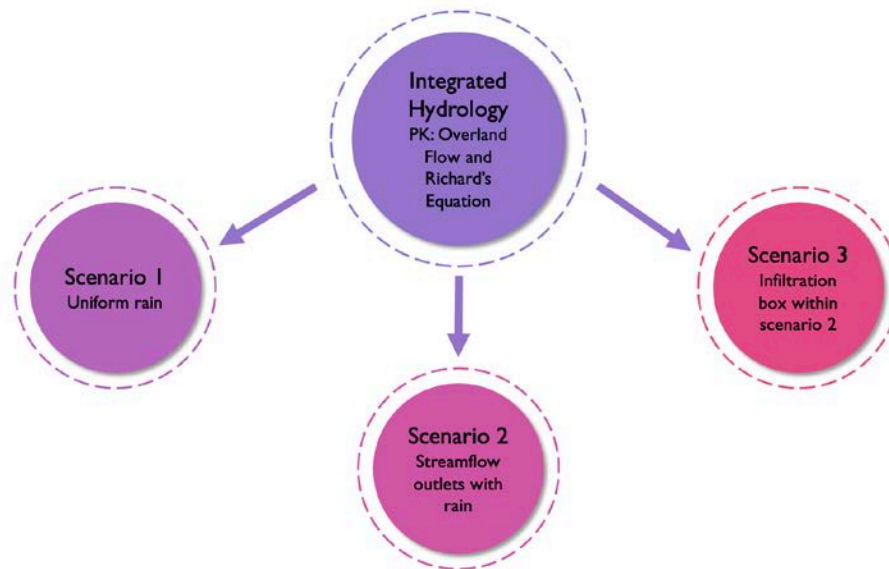
Figure 5. Scenarios that were developed for the understanding of coupled subsurface and surface flow.

An ATS input file for surface-only flow uses one process kernel (PK), which is overland flow. If one wants to evaluate the interaction between the surface and subsurface, then at least two process kernels are necessary. For the scenarios above, overland flow and Richard's Equations were coupled as described above. Three scenarios were determined, as seen in Figure 5. Each scenario builds upon the last, with scenario one being the simplest and scenario three being the most complex. Scenario one is a hydrology simulation with uniform rain across the region, also known as the surface domain. Scenario two then adds to this input file by specifying the outlet set generated in TINerator. Scenario three finally combines the uniform rain and outlet with the addition of a square on the surface to analyze infiltration into that square. This is done by identifying boxes with coordinates, then specifying these boxes in the ATS input file as a region. Once a box is defined as a region, one can get more data on the infiltration within that box. Below is the ATS input file for scenario three, which includes uniform rain, the outlet point, and different soil types.

```xml
<!-- Begin: Regions -->
<ParameterList name="regions" type="ParameterList">

  <ParameterList name="computational domain" type="ParameterList">
    <ParameterList name="region: all" type="ParameterList">
    </ParameterList>
  </ParameterList>
  <ParameterList name="surface domain" type="ParameterList">
    <ParameterList name="region: all" type="ParameterList">
    </ParameterList>
  </ParameterList>


  <ParameterList name="top layer" type="ParameterList">
    <ParameterList name="region: labeled set" type="ParameterList">
      <Parameter name="label" type="string" value="1" />
      <Parameter name="file" type="string" value="../data/borden_mesh_coarse.exo" />
      <Parameter name="format" type="string" value="Exodus II" />
      <Parameter name="entity" type="string" value="Cell" />
    </ParameterList>
  </ParameterList>
  <ParameterList name="middle layer" type="ParameterList">
    <ParameterList name="region: labeled set" type="ParameterList">
      <Parameter name="label" type="string" value="2" />
      <Parameter name="file" type="string" value="../data/borden_mesh_coarse.exo" />
      <Parameter name="format" type="string" value="Exodus II" />
      <Parameter name="entity" type="string" value="Cell" />
    </ParameterList>
  </ParameterList>
  <ParameterList name="bottom layer" type="ParameterList">
    <ParameterList name="region: labeled set" type="ParameterList">
      <Parameter name="label" type="string" value="3" />
      <Parameter name="file" type="string" value="../data/borden_mesh_coarse.exo" />
      <Parameter name="format" type="string" value="Exodus II" />
      <Parameter name="entity" type="string" value="Cell" />
    </ParameterList>
  </ParameterList>

  <!-- ATS extracts the surface boundary (as a handy default option) from your mesh -->
  <ParameterList name="surface boundary" type="ParameterList">
    <ParameterList name="region: boundary" type="ParameterList">
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Figure 6. Region definitions in the ATS input file for the surface, boundary, and top layer.

The first step in developing the ATS input file was to define the mesh and regions. The mesh is the ExodusII file developed with TINerator, and defining it means to direct ATS to the file path. When the mesh was created in TINerator, sets were developed with numerical labels. These labels are used in the region section of an ATS input file to specify what each set is. The region definitions in the input file are seen in Figure 6, Figure 7 and Figure 8.

The first region that needs to be defined is the surface domain, which is the entire surface of the mesh, including the boundary of the mesh. The surface domain and boundary are defined by name in TINerator as "all" for the surface domain and "boundary" for the surface boundary. The surface boundary is defined at the bottom of the figure above. The layers developed in TINerator are also defined in the above figure, with the top layer being 1, the middle layer as 2, and the bottom layer as 3. These labels show ATS where each layer is in the mesh file. Once these sets are defined as "regions", subsequent references to define parameters or boundary conditions, for example, can use the names the user has chosen as opposed to the less intuitive numbers.

```
<!-- Outlet on the surface, derived from the 3D mesh -->
<ParameterList name="stream outlet" type="ParameterList">
  <ParameterList name="region: labeled set" type="ParameterList">
    <Parameter name="label" type="string" value="31" />
    <Parameter name="file" type="string" value="../data/borden_mesh_coarse.exo" />
    <Parameter name="format" type="string" value="Exodus II" />
    <Parameter name="entity" type="string" value="face" />
  </ParameterList>
</ParameterList>

<ParameterList name="subsurface outlet" type="ParameterList">
  <ParameterList name="region: labeled set" type="ParameterList">
    <Parameter name="label" type="string" value="31" />
    <Parameter name="file" type="string" value="../data/borden_mesh_coarse.exo" />
    <Parameter name="format" type="string" value="Exodus II" />
    <Parameter name="entity" type="string" value="face" />
  </ParameterList>
</ParameterList>

<ParameterList name="boundary_except_outlet" type="ParameterList">
  <ParameterList name="region: labeled set" type="ParameterList">
    <Parameter name="label" type="string" value="30" />
    <Parameter name="file" type="string" value="../data/borden_mesh_coarse.exo" />
    <Parameter name="format" type="string" value="Exodus II" />
    <Parameter name="entity" type="string" value="face" />
  </ParameterList>
</ParameterList>
```

Figure 7. Region definitions in the ATS input file for the outlet.

The next item to be defined is the surface and subsurface outlet. The outlet was created in TINerator as a set, in which a label number was automatically generated. This is different from the layers described in Figure 6. The label number for the outlet is "31," and the name given to the outlet is "stream outlet" and "subsurface outlet." The names for the surface and subsurface outlets are used later in the input file to create "observations" in which the outlet data will be recorded for more in-depth analysis.

```
<!-- infiltration region define -->
<ParameterList name="infiltration_box" type="ParameterList">
  <ParameterList name="region: box" type="ParameterList">
    <Parameter name="low coordinate" type="Array(double)" value="{38, 2}" />
    <Parameter name="high coordinate" type="Array(double)" value="{45.0739, 3}" />
  </ParameterList>
</ParameterList>

<ParameterList name="infiltration_face" type="ParameterList">
  <ParameterList name="region: logical" type="ParameterList">
    <Parameter name="operation" type="string" value="intersect" />
    <Parameter name="regions" type="Array(string)" value="{surface domain, infiltration_box}" />
  </ParameterList>
</ParameterList>
```

Figure 8. Region definitions in the ATS input file for the infiltration points.

Also defined in the region section is the infiltration face set. Infiltration can be analyzed later to visualize the amount of water entering the subsurface over time. To create an infiltration face set for this test case the option to use geometric objects to define sets, as well as the ability to apply mathematically logical operations on sets, are used. First, a box with a low and high coordinates

is defined, and then the "logical" intersection operation is used to intersect the surface domain and the infiltration box. This creates the face set named "infiltration_face".

```xml
<!-- Top-level execution control -->
<ParameterList name="cycle driver" type="ParameterList">

  <Parameter name="start time" type="double" value="0.0" />
  <Parameter name="start time units" type="string" value="s" />
  <Parameter name="end time" type="double" value="0.5" />
  <Parameter name="end time units" type="string" value="d" />
```

Figure 9. Defining the simulation run time.

An important part of an ATS input file is defining the length of the simulation, which ATS controls in the "cycle driver" XML section. This is shown in Figure 9, where the cycle driver was specified as half a day, or 12 hours. This was the time used for the Borden watershed simulation.

```xml
<!-- Rain-fall:
          - time = [0,6][h]
          - rate 20 [mm/h] = 5.556e-6 [m/s]  - very heavy rain, or heavy shower
          - (rain fall rate: subjective names https://water.usgs.gov/edu/activity-howmuchrain-metric.html)
     -->
<ParameterList name="surface-water_source" type="ParameterList">
  <Parameter name="field evaluator type" type="string" value="independent variable" />
  <Parameter name="constant in time" type="bool" value="true" />
  <ParameterList name="function" type="ParameterList">
    <ParameterList name="domain" type="ParameterList">
      <Parameter name="region" type="string" value="surface domain" />
      <Parameter name="component" type="string" value="cell" />
      <ParameterList name="function" type="ParameterList">
        <ParameterList name="function-tabular" type="ParameterList">
          <Parameter name="x values" type="Array(double)" value="{0.0,21600}" />
          <Parameter name="y values" type="Array(double)" value="{5.556e-06,0.0}" />
          <Parameter name="forms" type="Array(string)" value="{constant}" />
        </ParameterList>
      </ParameterList>
    </ParameterList>
  </ParameterList>
</ParameterList>
```

Figure 10. Defining the uniform rain in the ATS input file.

The surface water source tells ATS where the water for the surface flow is originating from and how much water is being input. Uniform rain is when there is a start and stop time of rain at a constant intensity for that period. The intensity is in units of meters per second. A heavy rain shower was used for the Borden watershed simulation at 22 mm/hr. The period of rain for the Borden watershed simulation was chosen to be 6 hours, with the entire simulation being 12 hours, as described above.

```xml
<!-- Begin: Observations -->
 <ParameterList name="observations" type="ParameterList">
 <!-- Outlet Observations-->
   <ParameterList name="subsurface outlet flux" type="ParameterList">
    <Parameter name="variable" type="string" value="mass_flux" />
    <Parameter name="direction normalized flux" type="bool" value="true" />
    <Parameter name="region" type="string" value="subsurface outlet" />
    <Parameter name="functional" type="string" value="extensive integral" />
    <Parameter name="delimiter" type="string" value=" " />
    <Parameter name="location name" type="string" value="face" />
    <Parameter name="write interval" type="int" value="1" />
    <Parameter name="observation output filename" type="string" value="subsurface_outlet_flux.dat" />
    <Parameter name="times start period stop" type="Array(double)" value="{0.0,7200,-1.0}" />
  </ParameterList>
  <ParameterList name="surface outlet flux" type="ParameterList">
    <Parameter name="variable" type="string" value="surface-mass_flux" />
    <Parameter name="direction normalized flux" type="bool" value="true" />
    <Parameter name="region" type="string" value="stream outlet" />
    <Parameter name="functional" type="string" value="extensive integral" />
    <Parameter name="delimiter" type="string" value=" " />
    <Parameter name="location name" type="string" value="face" />
    <Parameter name="write interval" type="int" value="1" />
    <Parameter name="observation output filename" type="string" value="surface_outlet_flux.dat" />
    <Parameter name="times start period stop" type="Array(double)" value="{0.0,600,-1.0}" />
  </ParameterList>
<!-- Infiltration Observations-->
<ParameterList name="surface infiltration" type="ParameterList">
    <Parameter name="variable" type="string" value="surface-mass_flux"/>
    <Parameter name="direction normalized flux" type="bool" value="true" />
    <Parameter name="region" type="string" value="infiltration_face" />
    <Parameter name="functional" type="string" value="extensive integral" />
    <Parameter name="delimiter" type="string" value=" " />
    <Parameter name="location name" type="string" value="face" />
    <Parameter name="write interval" type="int" value="1" />
    <Parameter name="observation output filename" type="string" value="surface_infiltration.dat" />
    <Parameter name="times start period stop" type="Array(double)" value="{0.0,3600.0,-1.0}" />
  </ParameterList>
</ParameterList>
<!-- End: Observations -->
```

Figure 11. Adding Observations for the Outlet and Infiltration Face.

The observation section of the ATS input file creates data files to record the time series of specified quantities of interest over specific regions. Therefore, with an outlet on the Borden watershed, an observation was created so that the runoff from the outlet would be recorded in the data file. The data file can then be plotted using tools such as matplotlib in python. The same approach applys to the infiltration face, where the amount of rainwater infiltrating the specified region can be recorded.

2.2.3 Visualization of the Borden Watershed

Visualization occurs after the ATS input file has been run in the terminal. ATS will generate multiple visualization files that can be opened in VisIt or ParaView. In the visualization, the model created by TINerator, which comprises both the mesh and labeled sets, is displayed. In addition, the both parameter (e.g., permability) and solution fields (e.g., subsurface saturation) are contatined in the visualization files and can be displayed on the mesh. In the internship, the surface ponded depth and subsurface liquid saturation were the most common fields visualized with these tools. In the figure below, one can see the Borden watershed being visualized using VisIt. The figure displays an image from a video simulation in the first hour of the simulation. The surface layer was given a "water-brown" color scheme. This color table is used to show the ponded depth of water along the surface after six hours of rain over the 12-hour period. The brown represents no

ponded water along the surface, and the darker the blue color, the more water is ponded. The surface layer was transformed upward in the z-direction for the visualization to show what is happening in the subsurface for saturation. The subsurface uses a multicolor table to show saturation. The warmer the color, the more saturation of the subsurface, and the cooler the color, the less to no saturation.

Figure 12. Image from the visualization of the Borden watershed taken at the first hour of the 12-hour simulation. The visualization displays the surface ponded water depth and the subsurface saturation.

The rain begins at time zero and ends after six hours. The simulation shows that water ponds on the surface in the first hour of the simulation during the rainfall. The subsurface becomes highly saturated along the stream in the first hour of rainfall. After six hours the rainfall stops and the visualization then shows the ponded water depth decreasing along the stream. The subsurface stays highly saturated for the entire 12 hours because the subsurface domain had no-flow boundary conditions. These results can be verified in the data files generated from infiltration and the runoff from the outlet.
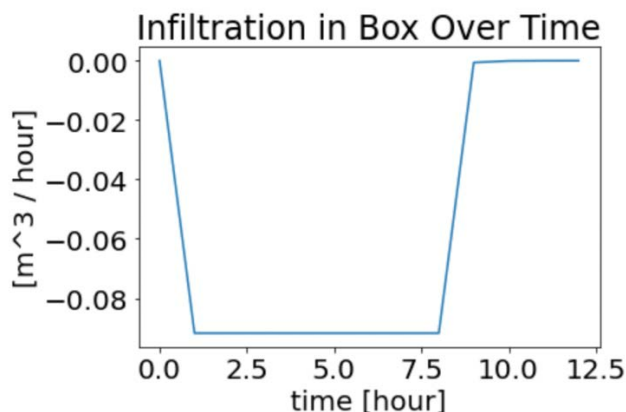
Figure 13. Plot generated in python for the infiltration.

In Figure 13, a plot was made in python from the output data file generated by ATS. As described above, in the observation section of the ATS input file, ATS was directed to give an output file listing data calculated for the surface infiltration into the infiltration face for the 12-hour simulation. In the infiltration plot, the infiltration increased in the first two hours of the simulation. Maximum infiltration occurred after seven and a half hours, after which the infiltration decreased back to the starting point. The rain in the simulation runs from zero to six hours, and the infiltration follows this timeline. When the rain stops after six hours, the infiltration stops soon after as there is no further input into the surface besides the ponded water after six hours.
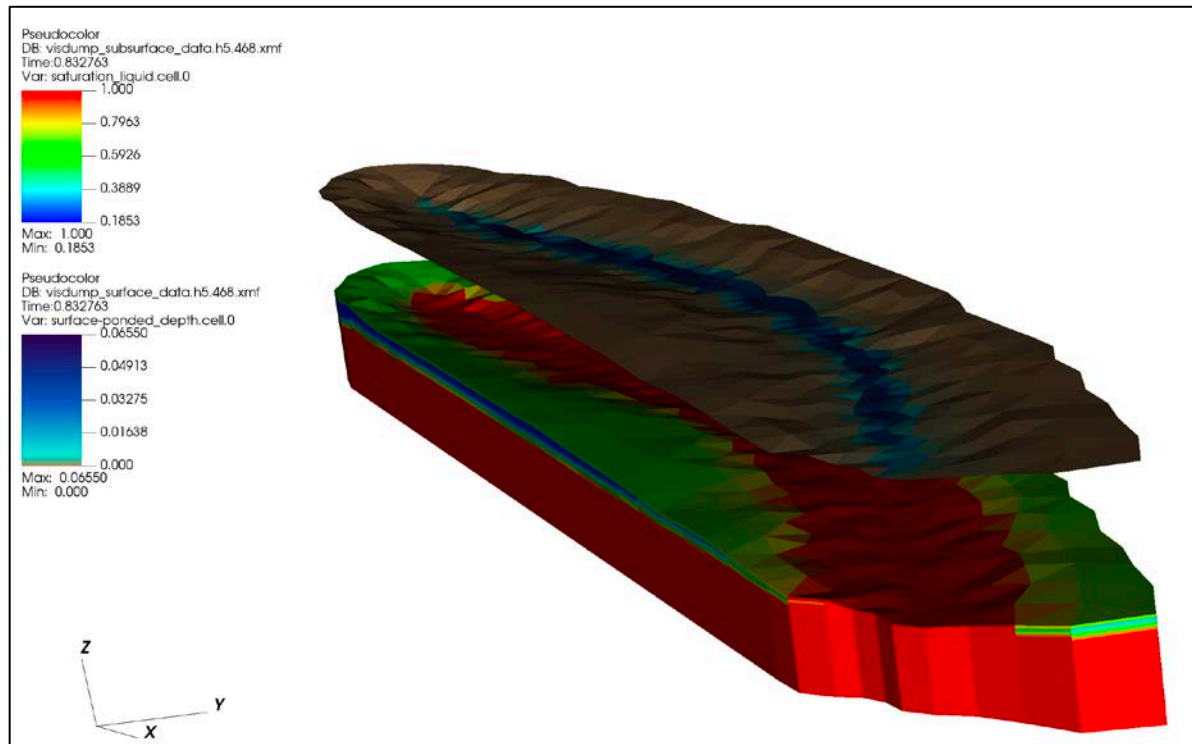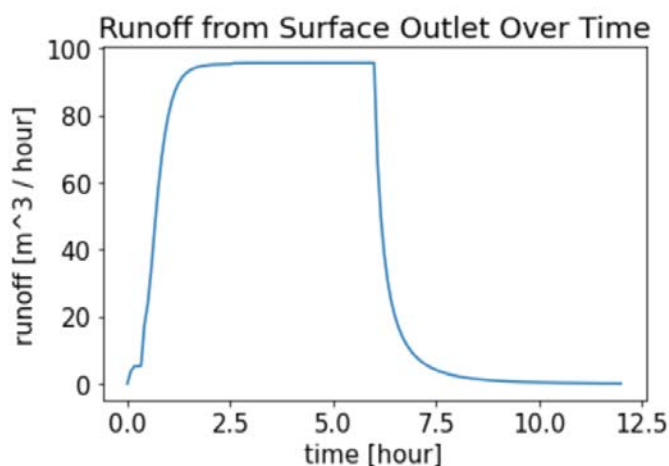

Figure 14. Image from the visualization of the Borden watershed taken at the first hour of the 12-hour simulation. The visualization displays the surface ponded water depth and the subsurface saturation.

In Figure 14, the runoff from the Borden watershed outlet is plotted using the data file generated from ATS. This data file was generated the same way as the infiltration data file. The runoff from the outlet increased dramatically as the rain fell in the watershed, then the runoff slowed directly after the rain ended after six hours. The plot shows the maximum runoff from the outlet over the 12 hours at 95 m^3/hr. There was no runoff at 12 hours of simulation time.

3. RESULTS AND ANALYSIS

After the methodology for developing an integrated hydrology model using TINerator and ATS was established, the workflow was then applied to a sub-basin of Basin 6. A sub-basin was used instead of the entire Basin 6 to work on a smaller scale. A smaller scale project would facilitate faster run times in order to complete the scope of the training particularly given the time constraint of the internship. The scope of the internship was to learn ATS and the workflow using practice areas; applying ATS to the entire Basin 6 was outside the scope.

Before the internship, a high-resolution (1-meter) digital elevation model (DEM) was developed using the United States Geological Survey (USGS) as a data source. A watershed delineation using ArcHydro was performed and sub-basins were identified, two of which can be seen in Figure 15. For the internship, a small and simple sub-basin was chosen from the work done by FIU
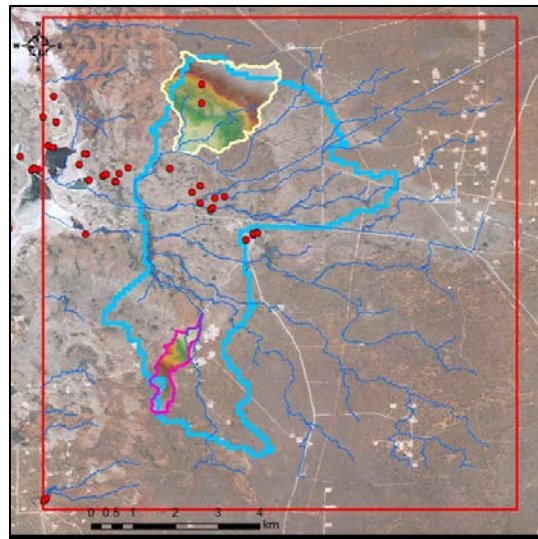

Figure 15. Aerial image of the Basin 6 study area (blue outline) with sinkholes (red points), the sub-basin selected for the internship (yellow outline), and another sub-basin delineated by FIU (pink outline).

The area outlined in yellow is the sub-basin that was chosen for the internship work, particularly as there were sinkholes (red points in the above figure) identified in that area, which the second sub-basin outlined in pink did not contain. This gave the DOE Fellow an opportunity to practice adding sinkholes into an ATS simulation. The shapefile for the sinkholes was obtained from a study done to identify and map the sinkholes in the Nash Draw (Goodbar et al., 2020).

3.1 Workflow of the Model Development for a Sub-Basin of Basin 6

3.1.1 Generating the Mesh and Sets for a Sub-Basin of Basin 6

To create an ExodusII unstructured mesh for the sub-basin, the 1-meter DEM and the sinkhole shapefile for the region in Basin 6 were imported into a JupyterLab Python file. This Python file is where the Python module, TINerator, is used. The DEM and sinkhole plot for the sub-basin (Sub-basin 2) can be seen in Figure 16, and the corresponding code can be seen in Figure 17.
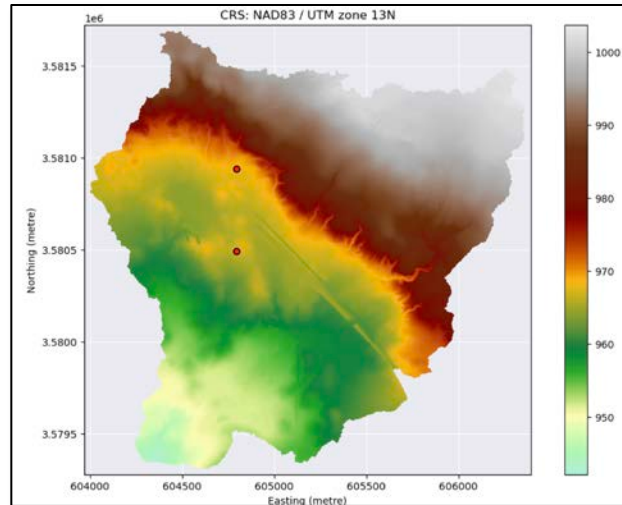
Figure 16. JupyterLab plot generated of the Sub-basin 2 DEM along with mapped sinkholes in the region.

```python
dem = tin.gis.load_raster("../../data/dem/Sub-Basin2a_DEM.tif", no_data=-9999.0)
dem.data[dem.data<=0]=-9999.0
dem.data[dem.data>1e5]=-9999.0
dem = tin.gis.reproject_raster(dem,"EPSG:26913")
#dem.no_data_value = dem.data[0][0]
dem.fill_depressions()
# +units=m +no_defs
print (dem.data[0,0])

sinkhole = tin.gis.load_shapefile("../../data/sinkholes/SinkholeAndrea_Basin6.shp")

sinkhole.plot(layers=[dem])
```

Figure 17. Code added to JupyterLab to import the DEM and sinkholes using TINerator.

After importing the DEM and sinkholes of Sub-basin 2, a watershed delineation was performed following the same procedure as described above in Section 2.2.1 Generating the Mesh and Sets for the Borden Watershed. In this case a threshold value of 80,000 was used. The delineated watershed and the corresponding code are seen in Figure 18 and Figure 19 below.

Figure 18. Script directing TINerator to perform a watershed delineation.
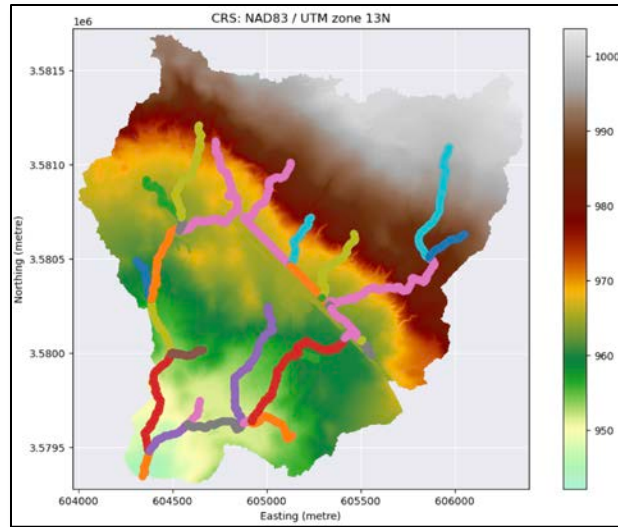
Figure 19. JupyterLab plot generated of the Sub-basin 2 DEM after the watershed delineation.

Then, an unstructured, triangulated mesh was generated. The mesh was created using the same methodology as the Borden watershed case, in which the minimum and maximum edge lengths were chosen for the mesh. The minimum edge length was 0.005 meters, and the maximum was 0.05 meters. Three layers, each one meter in thickness, were then added to the mesh. The code for creating the mesh is seen in Figure 20. The mesh for the sub-basin is displayed in Figure 21.

```
triangular_surface = tin.meshing.triangulate(
    dem,
    min_edge_length=0.005,
    max_edge_length=0.05,
    method='meshpy',
    refinement_feature=ws_flow,
    scaling_type='relative',
)

triangular_surface.view(window_size=(400,400))


layers = [
    ("constant", 0.5, 5, 1),
    ("constant", 1., 5, 2),
    ("constant", 5, 5, 3),
]

vol_mesh = tin.meshing.extrude_mesh(triangular_surface, layers)
vol_mesh.view(window_size=(800,800))
```

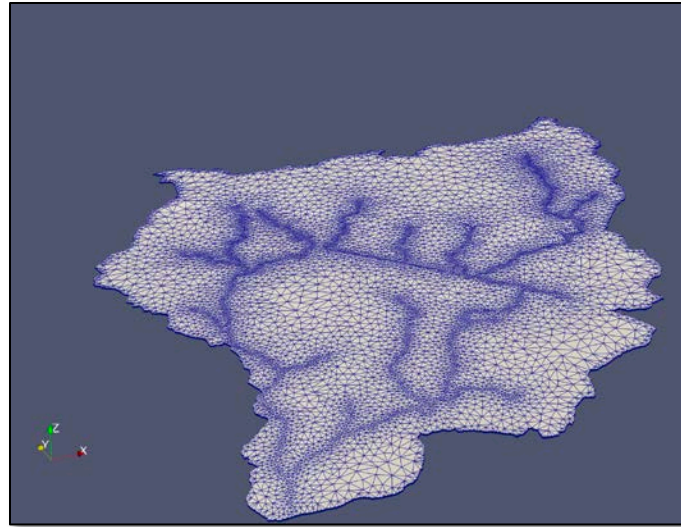**Figure 20. The TINerator code in JupyterLab that generated the mesh.**

Figure 21. The unstructured triangulated mesh generated for Sub-basin 2.

After the surface mesh and layers have been created, sets in the mesh can be identified. The first sets identified are the top, middle, bottom face, and domain boundary. The next set to be identified are the sinkholes. There are two sinkholes present in the sub-basin. A geometry function is used to create the sinkhole set since the sinkholes are from a polygon shapefile. Another set to be generated is the outlet. The coordinates for a left end and a right end were specified to create the outlet. These points were chosen after viewing the watershed delineation and determining where the water would exit the sub-basin. The code for creating the sets is seen in Figure 22, and the mesh sets are seen in Figure 23.

```python
# Extract top and bottom faces, and side nodes
top_faces = surf.top_faces
bottom_faces = surf.bottom_faces
side_faces = surf.side_faces

print('Sets')
print('----')
print(top_faces)
print(bottom_faces)
print(side_faces)

# View them
vol_mesh.view(sets=(top_faces, bottom_faces, side_faces), window_size=(800, 800))

sinkhole_faceset = surf.from_geometry(sinkhole)
vol_mesh.view(sets=[sinkhole_faceset])

outlet_pts = [
    (604399, 3579340),
    (604304, 3579350),
]

# Returns list of two sets
outlet = surf.discretize_sides(
    outlet_pts, close_ends=True, #at_layer=(1, 1), set_name_prefix="Outlet"
)

outlet[0].name = None
outlet[1].name = None

top_faces.name = None
bottom_faces.name = None
sinkhole_faceset.name = None

vol_mesh.view(sets=[outlet],window_size=(800, 800))
```

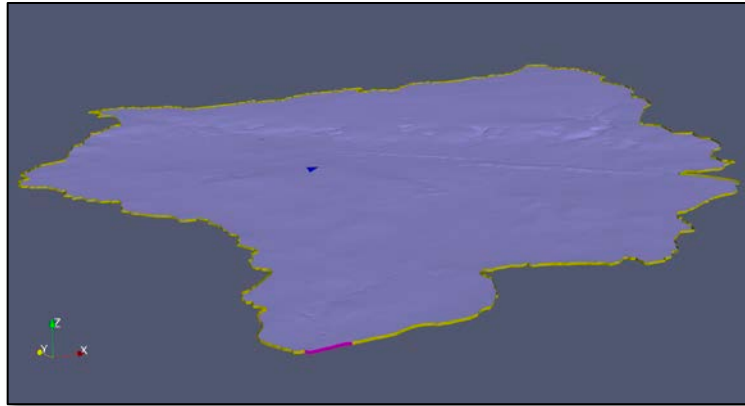**Figure 22. The code to generate sets for the mesh of the sub-basin.**

Figure 23. Visualization of the sets generated on the mesh for the sub-basin.

So that each set described above can be identified in the ATS input file, labels for each set were generated in TINerator. The labels for each set were:

- Sinkhole Geometry = 30 (blue color)
- Boundary = 31 (yellow color)
- Outlet = 32 (pink color)
- Top Face = 33 (purple color)
- Bottom Face =34 (not pictured)

3.1.2 Developing the ATS input file for the Sub-basin of Basin 6

To develop the ATS input file for the Sub-basin of Basin 6, the same methodology was used as for the Borden watershed described in Section 2.2.2 Developing the ATS Input File for the Borden Watershed; however, in this case the sinkholes set was also defined. Figure 24 shows the section of the ATS input file that defines the code. Since the code was a set, it is defined with the label "30".

```xml
<!-- Sinkhole Region -->
  <ParameterList name="sinkhole" type="ParameterList">
    <ParameterList name="region: labeled set" type="ParameterList">
      <Parameter name="label" type="string" value="30" />
      <Parameter name="file" type="string" value="../subbasin2_volume_mesh-meshpy-05-005_outlet.exo" />
      <Parameter name="format" type="string" value="Exodus II" />
      <Parameter name="entity" type="string" value="face" />
    </ParameterList>
  </ParameterList>
```

Figure 24. Defining the sinkholes in the region section of the ATS input file.

The next section of the ATS input file was to define the cycle driver, which controls the simulation time. The simulation time chosen was 12 hours. After the cycle driver, the process kernels (PKs) needed to be defined. This ATS input file used the same PK tree as the Borden watershed described in the methodology. Therefore, the PK section in the input file was copied from the Borden watershed, with the diffusive wave equation for the surface coupled with Richard's equation for the subsurface. After the PKs were defined in the input file, the water source was then scripted. The water source for the sub-basin simulation was heavy rain. Heavy rain was chosen as opposed

to light rain for the simulation as it best represented the Basin 6 region during the heavy monsoon season during the summer. The intensity chosen was 20 mm/h uniform over four hours. The heavy rain was set to start at time zero and end after four hours. Figure 25 shows the definitions for the sub-basin rainfall.

```
<!-- Rain-fall:
        - time [0,4][hours] = [0,14400][s]
        - rate 20 [mm/h] = 5.556e-6 [m/s]- very heavy rain, or heavy shower
        - (rain fall rate: subjective names https://water.usgs.gov/edu/activity-howmuchrain-metric.html)
    -->

<ParameterList name="surface-water_source" type="ParameterList">
  <Parameter name="field evaluator type" type="string" value="independent variable" />
  <Parameter name="constant in time" type="bool" value="true" />
  <ParameterList name="function" type="ParameterList">
    <ParameterList name="domain" type="ParameterList">
      <Parameter name="region" type="string" value="surface domain" />
      <Parameter name="component" type="string" value="cell" />
      <ParameterList name="function" type="ParameterList">
        <ParameterList name="function-tabular" type="ParameterList">
          <Parameter name="x values" type="Array(double)" value="{0.0,14400}" />
          <Parameter name="y values" type="Array(double)" value="{5.556e-06,0.0}" />
          <Parameter name="forms" type="Array(string)" value="{constant}" />
        </ParameterList>
    </ParameterList>
  </ParameterList>
```

Figure 25. Defining the rainfall in the 'region' section of the ATS input file.

After the rainfall is defined in the ATS input file, parameters relating to the geology of the region are added. Since there is limited soil data for the sub-basin of Basin 6, soil data from the Borden watershed was used. The table below displays important elements used in the ATS input file and the data sources. The sinkholes defined earlier were given a different surface Manning coefficient from the surface domain. This was done to expand on ATS knowledge and the steps to differentiate various areas on the surface.

Table 1. Elements Defined in the ATS Input File for the Sub-basin of Basin 6.

Element	Value	Unit	Data Source
Cycle Driver	12	h	N/A
Water source (rain)	5.556e-06	m/s	https://water.usgs.gov/edu/activity-howmuchrain-metric.html
Water source cycle	4	h	N/A
Surface manning coefficient for the surface	0.07	N/A	https://www.engineeringtoolbox.com/mannings-roughness-d_799.html Earth Channel – Weedy
Surface manning coefficient for the sinkholes	0.03	N/A	Borden watershed (Kollet et al., 2017)
Permeability for the top layer	1.02e-12	H/m	Borden watershed (Kollet et al., 2017)
Permeability for the top layer	1.02e-13	H/m	Borden watershed (Kollet et al., 2017)

Permeability for the bottom layer	1.02e-14	H/m	Borden watershed (Kollet et al., 2017)

Once the soil elements have been specified in the ATS input file, the observations can then be stated, which will allow a data file to be created for a specific aspect. Like the Borden watershed, an outlet data file was specified so that the runoff from the outlet could be plotted and analyzed.

3.1.3 Visualization and Analysis of the Sub-basin of Basin 6

After the ATS simulation was performed, the results were visualized similarly to the Borden watershed case, using VisIt. The simulation was 12 hours, with four hours of rain starting at the beginning. The surface and subsurface were visualized, the surface ponded depth was visualized on the surface, and saturation was analyzed on the subsurface. Figure 26 shows an image from the visualization at the ninth hour of the simulation. This is five hours after the heavy rain has stopped.
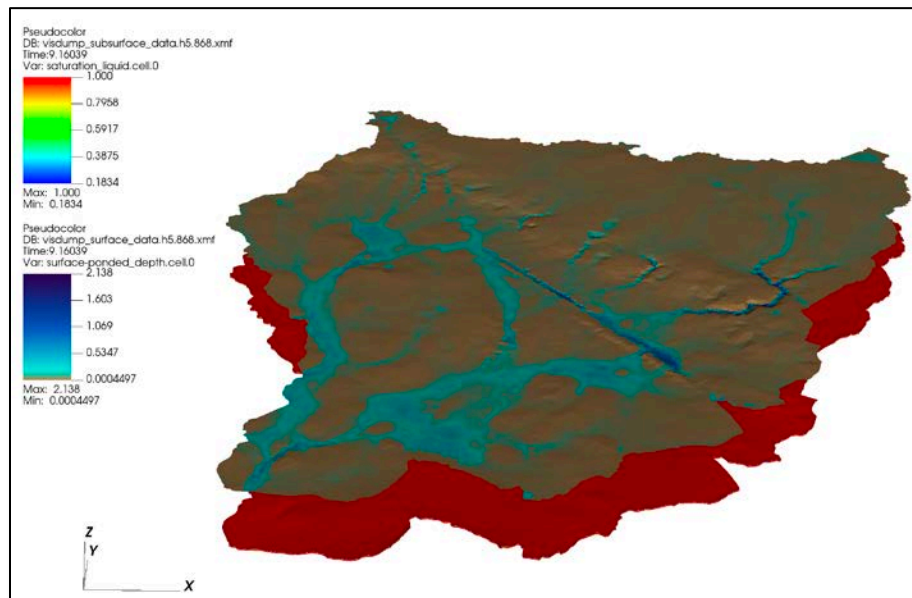

Figure 26. Image of the surface and subsurface visualization at the ninth hour of the simulation using VisIt.

In Figure 26, the visualization shows that the subsurface is still fully saturated, and water is still ponded on the surface five hours after the rain has stopped. The visualization also shows that the deepest ponded water is located at the outlet point and towards the middle of the sub-basin. When a satellite image was analyzed of the sub-basin region, a road can be seen going through the middle of the sub-basin, as seen in Figure 27.

In Figure 27, the red circle identifies the road that passes through the sub-basin. The water ponded up along the road as well as the lower outlet. This is because the road has a raised surface forming an obstruction to flow, while features like culverts or bridges that would preserve key connections in the drainage network are not represented in the DEM, and hence, are missing from the model.
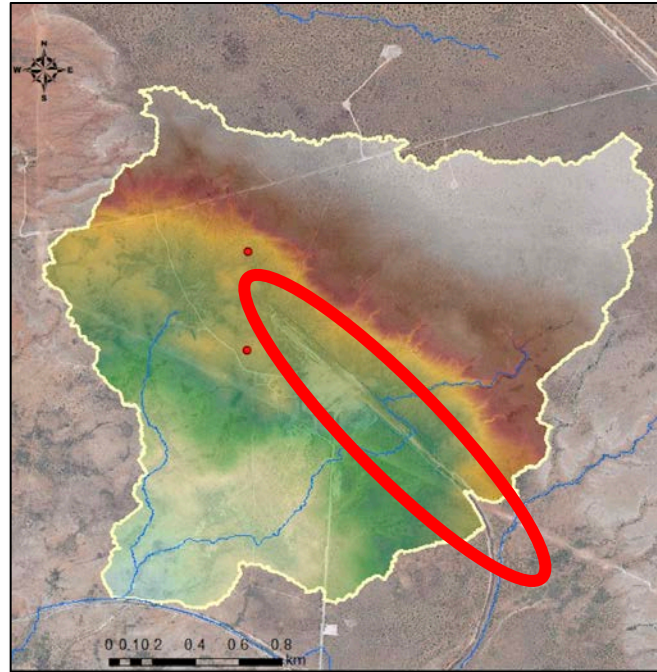
Figure 27. Satellite image showing the road (circled in red) that passes through the sub-basin.

The runoff from the surface outlet was plotted in python using the data file generated by ATS, as seen in Figure 28. The surface outlet runoff follows the trend of the rainfall, with the runoff decreasing after the rain has stopped. The maximum runoff from the outlet peaked at 4 million cubic meters per hour. The peak runoff occurred right after 4 hours, and drastically decreased right after as the rain stopped. This runoff is significantly larger than the runoff seen in the Borden watershed case, as it is a much larger area with more river network branch leading to the outlet.

The ATS model for the sub-basin brought to light many obstacles that still need to be investigated, including how to incorporate engineered features such as roads and bridges, as well as regional soil data into the ATS model, and how to more accurately portray the monsoon season within the model. These elements will all be evaluated moving forward with the model development. Despite the challenges encountered, the internship was impactful in understanding the workflow for generating an ATS integrated surface/subsurface hydrology model that can be applied to the entire Basin 6/Nash Draw study region.
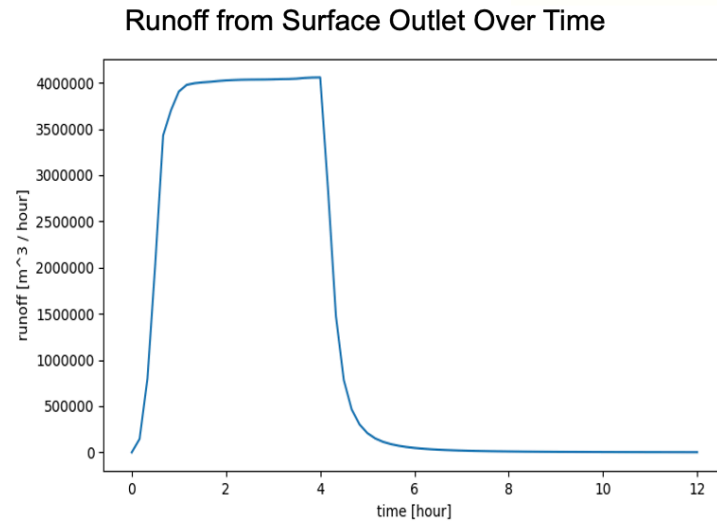
Figure 28. Plot of the runoff from the surface outlet of the sub-basin generated in python using ATS data files.

4. CONCLUSION

In conclusion, the internship not only helped to develop a greater understanding of the methodology behind generating an integrated surface/subsurface hydrology model using ATS, but it also emphasized some issues that need to be addressed for further development of the Basin 6 model. These include the need for more regional data, like soil parameters, vegetation types, regional geology, and meteorological data. It also showed the impact of engineered features such as roads in the area, and the need to determine how these surface features should be represented in the model. Overall, the internship provided greater knowledge and expertise in using the open-source software TINerator, ATS, VisIt, and ParaView. The Borden watershed example provided the backbone for the ATS input files that will continue to be used in the further development of the Basin 6 model. Moving forward, the skills learned during the internship will be applied to the Basin 6 work at Florida International University to study the impact of surface features on groundwater recharge and the rate of dissolution of the subsurface geological layers in the region of the WIPP.

5. REFERENCES

1. Chaturvedi, L. (1993). WIPP-related geological issues. In Carlsbad Region, New Mexico and West Texas, New Mexico Geological Society Forty-fourth Annual Field Conference, Carlsbad, NM (pp. 331-338).

2. Coon, E. T., Moulton, J. D., & Painter, S. L. (2016). Managing complexity in simulations of land surface and near-surface processes. Environmental modeling & software, 78, 134-149.

3. Goodbar, A. K., Powers, D. W., Goodbar, J. R., & Holt, R. M. (2020). Karst and sinkholes at Nash Draw, southeastern New Mexico (USA).

4. Kollet, S., Sulis, M., Maxwell, R. M., Paniconi, C., Putti, M., Bertoldi, G., ... & Sudicky, E. (2017). The integrated hydrologic model intercomparison project, IH-MIP2: A second set of benchmark results to diagnose integrated hydrology and feedbacks. Water Resources Research, 53(1), 867-890.

5. Livingston, D. (2020). TINerator API Reference. Los Alamos National Laboratory.