CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: FLOW-3D Training Courses
AI 06002.01.302.605

DATE AND PLACE: August 8–11, 2006
Santa Fe, New Mexico

AUTHOR: D. Basu, CNWRA
K. Das, CNWRA

DISTRIBUTION:

NRC	**CNWRA**	**SwRI**
W. Reamer	W. Patrick	Record Copy B, IQS
V. Whipple	B. Sagar	
D. DeMarco	GED Directors	
S. Kim	GED Asst. Directors	
J. Trapp	GED Managers	
J. Rubenstone	L. Gutierrez	
B. Hill		
P. Justus		
J. Guttmann		
R. Fedors		

CENTER FOR NUCLEAR WASTE REGULATORY ANALYSES

TRIP REPORT

SUBJECT: FLOW-3D Training Course
AI 06002.01.302.605

DATE/PLACE: August 8–11, 2006
Santa Fe, New Mexico

AUTHORS: D. Basu
K. Das

SENSITIVITY: Non-Sensitive

PERSONS PRESENT: Approximately seven participants attended the course.

BACKGROUND AND PURPOSE OF TRIP: FLOW-3D is a general purpose, fluid dynamics software that is widely used. It is primarily used for simulating flows with sharp interfaces or high density gradients, which are commonly referred to as free surface flows. In addition, FLOW-3D has multiphysics capability that simulates external and internal flows with complex geometries and widely varying flow properties. FLOW-3D solves the Navier-Stokes Equations using a Fractional Area Volume Obstacle Representation (FAVOR) approach, defining general geometric regions within the rectangular grid. The philosophy behind FAVOR is that numerical algorithms are based on information consisting of only one pressure, one velocity, one temperature, etc., for each control volume. Because using much more information to define the geometry would create inconsistencies, the FAVOR technique retains the simplicity of rectangular elements while representing complex geometric shapes at a level consistent with the use of averaged flow quantities within each volume element. The simplicity of the FAVOR method in FLOW-3D for modeling complex geometric regions is an attractive feature.

FLOW-3D has been used in computational fluid dynamics analyses by Southwest Research Institute staff members, especially for understanding the in-drift flow and thermal processes. The developer of FLOW-3D, Flow Science, Inc., offers a training program every 3 months for new users of this software. This 4-day training was held in Santa Fe, New Mexico. The first 3 days were spent demonstrating the capabilities of FLOW-3D and discussing the graphical user interface, theory, numerics, and other associated features of the software. Each day of training was divided into four sessions. Each session covered a particular aspect and was followed by simple hands-on demonstrations and exercises with representative problems. The final day focused on customization of the code, as well as discussion of specific problems by the participants.

The purpose of the trip was twofold: (i) to become accustomed with the details of the FLOW-3D software and establish contact with the support staff at Flow Science, Inc., and (ii) to evaluate the software's ability to analyze existing geologic, hydrologic, and engineering problems at Center for Nuclear Waste Regulatory Analyses (CNWRA). The evaluation specifically involved the customization of the solver that may be required to model these problems.

SUMMARY OF PERTINENT POINTS AND ACTIVITIES: The introductory lectures focused on interacting with the graphical user interface, while illustrating the different features of the solver pre-processor tools. The lectures covered the basic Volume of Fluids method and the fractional area–volume object representation approach unique to FLOW-3D. Generating grids and incorporating external geometry and grid files in FLOW-3D was also discussed. Incorporating the initial and boundary conditions in a physical problem was subsequently discussed, along with modeling techniques required for moving frame of reference. Each of these lectures was followed by some simple hands-on demonstrations.

The second day was mainly focused on the numerics and physics of the flow solver, including the turbulence models. All the physical models in FLOW-3D were explained with suitable examples. The hands-on examples included problems involving weir flow, two-fluids problems, and also some high-speed aerospace applications. The lectures focused on selecting the appropriate physical model and coupling techniques and using the post-processor effectively.

Details of the advanced multiphase models and other multiblock capabilities were explained on the third day. The support staff at FLOW-3D explained the advantages and problems of using the multiblock options. The multiphase models in FLOW-3D involving two fluids were explained in detail. Sample problems involving two fluids of varying densities were solved by the FLOW-3D support staff.

On the fourth and final day, CNWRA staff had the opportunity to discuss their own problems with the FLOW-3D support engineers. The final day was also used to interact with the support engineers at Flow Science, Inc. The interactions were quite helpful in addressing some of the problems on which CNWRA is currently working. CNWRA staff also discussed different issues related to the customization of the FLOW-3D solver.

CNWRA staff also discussed the emerging issue of the LINUX-based FLOW-3D computations. Issues related to the parallel computation using FLOW-3D, use of MPI/OPEN-MP, the compiler selection, and optimization of computing power were also discussed.

CONCLUSIONS: The training course was extremely beneficial for finding out how to use the FLOW-3D code. The introductory lectures provided a very good overview on how to interact with the graphical user interface and the pre-processor tools, while the advanced lectures provided very good insight into the capabilities of the solver. The hands-on demonstrations provided an opportunity to assess the range of problems that can be solved efficiently using FLOW-3D. The customization session helped in understanding the important modules of the solver and what is needed to modify the code for existing and new applications.

PROBLEMS ENCOUNTERED: None.

PENDING ACTIONS: None.

RECOMMENDATIONS: None.

SIGNATURES:

Debashis Basu — 8/28/2006
Debashis Basu
Research Engineer, CNWRA
Date

Kaushik Das — 8/28/2006
Kaushik Das
Research Engineer, CNWRA
Date

CONCURRENCE:

8/28/2006
John A. Stamatakos
Manager, Geology and Geophysics
CNWRA
Date

8/29/2006
Robert Lenhard
Manager, Hydrology
CNWRA
Date

8/29/2006
Gordon Wittmeyer
Asst. Director, Earth Sciences
CNWRA
Date