SOFTWARE REQUIREMENTS DESCRIPTION MAGMA REPOSITORY INTERACTION SIMULATION CODE (SHOCK)

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Software Requirement Description

Introduction

A complete code will be developed for two-dimensional simulations of the fluid dynamics that ensues when a dike with high-pressure volatile-rich magma encounters a repository drift at atmospheric pressure. The overall goal is to calculate the pressure distribution at the roof of the repository drifts after magma breaks through from a dike into a drift. This code will extend the one-dimensional analyses performed previously (Bokhove and Woods, 2000). The following assumptions will be made in developing the code.

1. Since the waste canisters in the drift occupy a small cross-sectional area relative to the drift area, their influence on the fluid dynamics is neglected. This assumption will be expored with alternative geometries.

2. The multi-phase volatile-rich magma in the dike and the air in the drift is modeled as a pseudo two-phase fluid, in which the mass fractions of the liquid phase (liquid lava and water) and gas phase (water vapor or air) are dependent on an average pressure. The computational task then consists of modeling a compressible gas mixture with parameterized frictional forces. The large initial pressure differences result in high-speed gas-dynamics flows in which shock and rarefaction waves are resolved in a complex two-dimensional geometry (see Bokhove and Woods, 2000).

3. The complex three-dimensional geometry is simplified by averaging over one spatial dimension. The resulting equations of motion are then two-dimensional.

Software Function

The two-dimensional numerical code will be able to simulate leading-order magma interactions in a dike-drift geometry.

Theoretical Basis

The ensuing high-speed compressible magma flows are calculated by discretizing the multi-phase gas dynamics model with modern gas dynamics methods used in compressible and incompressible aerodynamics. Three methods will be investigated, including, Local Lax Friedrichs and Central Difference Essentially Non-Oscillatory (ENO) numerical schemes (Shu and Osher, 1989, Liu and Osher, 1998, Jiang et al, 1998). The best of these methods in terms of accuracy, speed and robustness will be used for the parameter study.The code will solve the convervation equations using a finite difference scheme. The equations solved are:

$$\frac{\partial(\rho\beta)}{\partial t}+\frac{\partial}{\partial x}(\rho u\beta)+\frac{\partial}{\partial z}(\rho w\beta)=0$$

$$\frac{\partial(\rho w\beta)}{\partial t}+\frac{\partial}{\partial x}(\rho uw\beta)+\frac{\partial}{\partial z}(\frac{1}{2}\rho w^2\beta+p\beta)=p\frac{\partial\beta}{\partial z}-\rho\beta g-F^{(z)}$$

$$\frac{\partial(\rho u\beta)}{\partial t}+\frac{\partial}{\partial x}(\frac{1}{2}\rho u^2\beta+p\beta)+\frac{\partial}{\partial z}(\rho uw\beta)=p\frac{\partial\beta}{\partial x}-F^{(x)}$$

with density $\rho=\rho(p)$, velocity (u,w) in the x,z direction, presusre p, gravitational acceleration g, fricitional dissipation terms $F^{(x)}$, $F^{(z)}$ in the x and z directions, and $\beta(x,z)$ is the lateral width of the dike/drift after averaging in the y -direction.

Similar equations appear when averaging is used in the dike in the x-direction. The geometry of the dike and drift will be fixed for individual runs. Nevertheless, as coupling between fluid pressure, flow and rock deformation exists, provision will be made in the code to allow this geometry to vary in a simple, smooth manner, as a function of time.

Computational Approach

The computer code will be written in the C-language in Ansi-C standard and operate on a variety of platforms (HP9000, Sun workstation, Linux PC's) with the different associated compilers (e.g. gcc and cc). The discretization methods include both finite-difference and finite-volume methods with predictor-corrector or Total Variation Diminishing time discretization schemes (Shu and Osher, 1989). Code validation is ensured by comparisons with exact solutions (in one- and two dimensions) and by comparing simulation resulting from different numerical algorithms.

Data Flow

Input text files will be used to provide the nescessary input parameters to the code. Format of these files will be such that they can be edited in any standard text editor. File format will be specified in the User's Manual along with example inputs. Results will be written to an output file in fixed format. The User's manual will describe the format of the output, which will be suitable for plotting using standard graphics packages.

Hardware and Software Requirements

Simulations of about 96000 degrees-of-freedom and tens of seconds are very manageable on a 450 MHz computer, although more high-resolution simulations require faster processors. Pre-processing consists of editing the input file, and post-processing consists of graphing the output files with standard graphics packages (e.g., Matlab, Tecplot).

References

Bokhove, O., and Woods, A.W. Explosive magma-air interactions by volatile-rich basaltic melts in a dike-drift geometry. Report to U.S. Nuclear Regulatory Commission. 2000.

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