

PLEASE READ THE FOLLOWING BEFORE USING THE RT3D CODE

RT3D (Reactive Transport in 3-Dimensions) is a finite-difference numerical code for simulation of three-dimensional, multi-species reactive transport in groundwater aquifers. RT3D comes with 7 built-in reaction kinetics modules, but also has the flexibility to utilize reaction mechanisms of any complexity that are defined by the user. RT3D calculates the reactive transport using the flow solution from a finite difference groundwater flow package such as MODFLOW. RT3D may be applied to a wide variety of reactive flow and transport scenarios, including accelerated *in situ* bioremediation system design, natural attenuation evaluation, and *in situ* chemical oxidation.

LICENSE AND COPYRIGHT INFORMATION

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DISCLAIMER OF WARRANTY

The RT3D computer code is provided without any warranty. We make no warranties, expressed or implied, that the RT3D code is free of errors or whether it will meet your need for solving a particular problem. You use the code at your own risk. The developers disclaim all liability for direct or consequential damage resulting from your use of the code.

CONTACT INFORMATION

There are several resources for RT3D users. The official RT3D web site provides information on features, manuals, downloads, and utilities. Several of the developers of groundwater modelling packages that have authorized RT3D interfaces (e.g., GMS, Visual Modflow, etc.) have support forums accessible thorough their respective web sites. If those resources do not provide the answers you seek, contact information is provided below.

General questions on RT3D use, functionality, documentation, etc. should be directed to Christian Johnson. Complex questions, "wish list" requests, and RT3D project related inquires should be directed to Dr. Clement. Contact Christian Johnson for discussion of how Battelle may assist your project with customized reaction modules, accelerated *in situ* remediation design, and/or natural attenuation evaluations.

Official RT3D Web Site: <http://bioprocess.pnl.gov/rt3d.htm>

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DOWNLOADING INSTRUCTIONS:

RT3D (and related files) may be downloaded from: <http://bioprocess.pnl.gov/rt3d.htm>

The files are available as a Windows zip file or a UNIX tar file. Once the zip or tar file is downloaded, move the file to an appropriate (working) directory, and decompress it using your favorite utility (e.g., "pkunzip -d rt3dall.zip" using PKZip from a command prompt). Select the appropriate option to restore the full directory structure. This will install the following files/directories. Files for Windows/Intel-x86 platforms are not included in the UNIX tar archive.

rt3dv25_readme.txt	This file (also in the Documentation folder as RT3Dv25_Readme.pdf).
<rt3d_exe>	Directory containing pre-compiled binaries for Intel x86/Windows systems. Includes rt3dv25.exe (no user-defined reaction), rt3dbat1.exe, rt3dv25dll.exe, rxns.dll, and jacrxns.dll files (the latter 3 files allow for user-defined reaction definitions in user-compiled DLL files, the files provided are just dummy procedures). For an interface-specific RT3D executable, please visit the authorized GUI-vendor's web site.
<docs>	Directory containing RT3D documentation: RT3Dv25_Readme.pdf, RT3Dv25_Update.pdf, PNNL_11720_RT3Dv1_Manual.pdf, PNNL_11805_RT3D_Tutorial_for_GMS.pdf, Dual_Porosity_Reaction_Module.pdf, and NAPL_Reaction_Module.pdf. The latter two documents are white papers describing the corresponding reaction modules that may be implemented as user-defined reaction modules. The free Adobe Acrobat Reader (v. 5.0) is required to read these documents (available at http://www.adobe.com).
<rt3d_src>	Directory containing the RT3Dv2.5 source files.
<rxnpkg_src>	Directory containing source code for 10 reaction modules (in separate files) for use as user-defined reaction modules.
<rt3dbat_src>	Directory containing the RT3DBAT v. 1.0b source files. Differs from version 1.0 only in that the DLL option is no longer the default.
<examples>	Directory containing files for the two examples discussed in the RT3Dv1 manual.
<modflow_src>	Directory containing the MODFLOW executable and source files.

LIST OF SOURCE FILES:

Source Files for RT3D V2.5

This version of RT3D was developed using standard Fortran 90. The code can be compiled on both Windows and Unix operating systems. The code is organized into the following Fortran source files:

- 1) rt3dv25.f - Main driver for the rt3d code

- 2) adv30d.f - Advection package (identical to MT3DMS)
- 3) dsp30d.f - Dispersion package (identical to MT3DMS)
- 4) fmi30d.f - Flow model interface (identical to MT3DMS)
- 5) gcg30d.f - GCG Solver package (identical to MT3DMS)
- 6) btrrtv25.f - Basic transport package (minor modifications vs. MT3DMS)
- 7) ssmrtv25.f - Source sink mixing package (minor modifications vs. MT3DMS)
- 8) utlrv25.f - Utility package (minor modifications vs. MT3DMS)
- 9) rtrctv25.f - RT3D reaction package (unique to RT3D)
- 10) rteqnv25.f - RT3D pre-programmed reaction modules (unique to RT3D)
- 11) solver123.f - RT3D reaction solvers 1, 2 and 3 (unique to RT3D)
- 12) solver45.f - Dummy procedure for solver45.f. RT3D reaction solvers 4 and 5 are optional solver routines that cannot be distributed via the Internet because of copyright issues. If you need access to these solvers then please contact the developers.
- 13) rxns.f - Example RT3D user-defined reaction module
- 14) jacrxns.f - Jacobian routine for the example user-defined reaction module

Source Files for RT3DBAT

rt3dbatv1.f is a utility package for integrating user-defined, RT3D reaction modules in a batch mode (batch reactor analysis). It is a stand-alone code and should be compiled with rxns.f (jacrxns.f is not required).

User-Defined Reaction Package Source Files

The files in the RxnPkg_src directory are reaction modules broken out into separate files for use as user-defined reaction modules. These files may be re-named as rxns.f and compiled with RT3D (or compiled to a DLL). The files include:

- rxn3.f Standard reaction module #3
- rxn4.f Standard reaction module #4
- rxn5.f Standard reaction module #5
- rxn6.f Standard reaction module #6
- rxn7.f Standard reaction module #7
- dualpore.f Dual porosity reaction module; see Dual_Porosity_Reaction_Module.pdf for more details
- napl.f NAPL reaction module; see NAPL_Reaction_Module.pdf for more details
- rxn_Ex_2a.f Reaction module for Example 2 (method 1) of the RT3Dv1 manual
- rxn_Ex_2b.f Reaction module for Example 2 (method 2) of the RT3Dv1 manual
- rxn_Ex_2c.f Reaction module for Example 2 (method 3) of the RT3Dv1 manual

Source Files for RT3D-specific MODFLOW

The MODFLOW-96 executable and source to be used with RT3D v 2.5 are included in the zip file under the subdirectory Modflow. This MODFLOW source can also be downloaded from: <http://www.ecgl.byu.edu/software/gms/support/modelinfo.html>.

Note that if you wish to use MODFLOW 2000, you must do two things. First, compile MODFLOW 2000 and RT3Dv2.5 using the same compiler; the executable for MODFLOW 2000 distributed by the U.S. Geological Survey (<http://water.usgs.gov/software/modflow-2000.html>) is compiled with Lahey while the RT3Dv2.5 executable is compiled with Visual Fortran. Second, in the LMT6 input file, you must specify the "Standard" header (or use a blank file); see U.S. Geological Survey Open-File Report 01-82 for more details.

COMPILING RT3DV2.5

RT3D compilation was tested using the Compaq Visual Fortran (v6.1) compiler on an Intel x86-compatible machine with a Microsoft Windows operating system and using a UNIX Fortran 90 compiler on a DEC-Alpha workstation. The "make" files given below can be used for compiling on Intel x86/Windows or UNIX platforms. A make file is also included for building the DLL version of RT3D; once RT3D with the DLL option is initially compiled, then only the rxns.f and jacrxns.f files will need to be compiled in the future (i.e., if the user-defined reactions are changed). See the RT3Dv2.5 Update document for more discussion of the DLL option. Note that some lines below may appear in wrapped form and will need to be a single line in an ASCII text file.

Make file for Windows (Compaq Visual Fortran)

```
FILES = rt3dv25.obj utlrtv25.obj adv30d.obj dsp30d.obj ssmrtv25.obj
btnrtv25.obj gcg30d.obj rteqnv25.obj fmi30d.obj rtrctv25.obj solver123.obj
solver45.obj rxns.obj jacrxns.obj
rt3dv25.exe : $(FILES)
    df -fast $(FILES)
rt3dv25.obj : rt3dv25.f
    df -fast -c rt3dv25.f
utlrtv25.obj : utlrtv25.f
    df -fast -c utlrtv25.f
adv30d.obj : adv30d.f
    df -fast -c adv30d.f
dsp30d.obj : dsp30d.f
    df -fast -c dsp30d.f
ssmrtv25.obj : ssmrtv25.f
    df -fast -c ssmrtv25.f
gcg30d.obj : gcg30d.f
    df -fast -c gcg30d.f
btnrtv25.obj : btnrtv25.f
    df -fast -c btnrtv25.f
fmi30d.obj : fmi30d.f
    df -fast -c fmi30d.f
rtrctv25.obj : rtrctv25.f
    df -fast -c rtrctv25.f
rteqnv25.obj : rteqnv25.f
    df -fast -c rteqnv25.f
solver123.obj : solver123.f
    df -fast -c solver123.f
solver45.obj : solver45.f
    df -fast -c solver45.f
Rxns.obj : Rxns.f
    df -fast -c rxns.f
jacrxns.obj : jacrxns.f
    df -fast -c jacrxns.f
```

Make file for Windows (Compaq Visual Fortran) For the DLL Version of RT3Dv2.5

```
FILES = rt3dv25.obj utlrtv25.obj adv30d.obj dsp30d.obj ssmrtv25.obj
btnrtv25.obj gcg30d.obj rteqnv25.obj fmi30d.obj rtrctv25.obj solver123.obj
solver45.obj rxns.lib jacrxns.lib
rt3dv25dll.exe : $(FILES)
    df /exe:rt3dv25dll.exe -fast $(FILES)
#Uncomment the following 4 lines if you need to rebuild the rxns.lib and
jacrxns.lib files; only required if you do not have the *.lib files
#rxns.lib : rxns.f
#    df /LD rxns.f
#jacrxns.lib : jacrxns.f
#    df /LD jacrxns.f
rt3dv25.obj : rt3dv25.f
    df -fast -c rt3dv25.f
utlrtv25.obj : utlrtv25.f
    df -fast -c utlrtv25.f
adv30d.obj : adv30d.f
    df -fast -c adv30d.f
dsp30d.obj : dsp30d.f
    df -fast -c dsp30d.f
ssmrtv25.obj : ssmrtv25.f
    df -fast -c ssmrtv25.f
gcg30d.obj : gcg30d.f
    df -fast -c gcg30d.f
btnrtv25.obj : btnrtv25.f
    df -fast -c btnrtv25.f
fmi30d.obj : fmi30d.f
    df -fast -c fmi30d.f
rtrctv25.obj : rtrctv25.f
    df -fast -c rtrctv25.f
rteqnv25.obj : rteqnv25.f
    df -fast -c rteqnv25.f
solver123.obj : solver123.f
    df -fast -c solver123.f
solver45.obj : solver45.f
    df -fast -c solver45.f
```

Make file for UNIX

```
F90C = f90
OBJECTS = rt3dv25.o \
    utlrtv25.o \
    adv30d.o \
    dsp30d.o \
    ssmrtv25.o \
    btnrtv25.o \
    gcg30d.o \
    rteqnv25.o \
    fmi30d.o \
    rtrctv25.o \
    solver123.o \
    solver45.o \
    rxns.o \
    jacrxns.o
rt3dv25: $(OBJECTS)
    $(F90C) -o rt3dv25 $(OBJECTS)
rt3dv25.o: rt3dv25.f
```

```
    $(F90C) -c rt3dv25.f
utlrtv25.o: utlrtv25.f
    $(F90C) -c utlrtv25.f
adv30d.o: adv30d.f
    $(F90C) -c adv30d.f
dsp30d.o: dsp30d.f
    $(F90C) -c dsp30d.f
ssmrtv25.o: ssmrtv25.f
    $(F90C) -c ssmrtv25.f
btnrtv25.o: btnrtv25.f
    $(F90C) -c btnrtv25.f
gcg30d.o: gcg30d.f
    $(F90C) -c gcg30d.f
rteqnv25.o: rteqnv25.f
    $(F90C) -c rteqnv25.f
fmi30d.o: fmi30d.f
    $(F90C) -c fmi30d.f
rtrctv25.o: rtrctv25.f
    $(F90C) -c rtrctv25.f
solver123.o: solver123.f
    $(F90C) -c solver123.f
solver45.o: solver45.f
    $(F90C) -c solver45.f
rxns.o: rxns.f
    $(F90C) -c rxns.f
jacrxns.o: jacrxns.f
    $(F90C) -c jacrxns.f

#clean:
#    rm -f *.o
```