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3.8.2 Instructions for Performing the Test and Expected Results

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1.0 Background and Scope

The Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES) is a software platform for selecting and implementing environmental software models for risk assessment and management problems. The FRAMES User Interface (FUI) allows users to link, select, and interact with environmental models for environmental and human health analyses. The formulations for this module are provided in Whelan et al. 1997.

This document describes how the FRAMES Chemical Database Editor (CDBE) was tested to ensure it meets its requirements. The document lists the specific requirements of the FRAMES CDBE, shows how the test cases that follow relate to these requirements, describes each test case, and describes the results of running each test case. The test cases address the basic functionality listed in the requirements.

2.0 Requirements

The Requirements for the FRAMES Chemical Database Editor (CDBE) are described in the DRAFT document *Requirements for the FRAMES Chemical Database Editor*, Rev 8, dated 12/12/00, by D.L. Strenge.

Table 1. The Requirements for the FRAMES Chemical Database Editor

Requirement Number	Requirements for the FRAMES Chemical Database Editor
1	Operate within the FRAMES software system
2	Allow the user to create, access, and save a chemical database (.mdb file)
3	Allow the user to select an existing database from a list of available databases (in the FRAMES database format) to be used for an analysis
4	Allow the user to select a constituent for viewing or editing
5	Allow the user to select constituents from a list ordered by name or CAS ID
6	Allow the user to change any property value associated with the constituent
7	Allow the user to print a paper copy or write to a file, a report of properties for one or more constituents
8	<i>This requirement has been deleted:</i> Allow the user to create a delimited file of database parameters (e.g., CSV file) for selected constituents and properties
9	Provide help information about the parameters in the database
10	Provide error messages to the user when inappropriate values are provided for any parameter (as determined by ranges defined within the database).
11	Reworded to: Operate in Windows 95/98/NT
12	Not require modifications to any existing components that run under FRAMES (i.e., GENII and MEPAS)
13	Allow the user to assign references to each property value added or modified
14	Allow the user to add new references or select from previous references
15	Provide property estimation methods for selected properties [as in the Multimedia-Modeling Environmental Database Editor (MMEDE) software]
16	Allow the user to select or deselect constituents to be included in an analysis
17	Allow the user to view constituents grouped by chemical groups (e.g.,

Requirement Number	Requirements for the FRAMES Chemical Database Editor
	polycyclic aromatic hydrocarbons).
18	The user should also be allowed to add or delete contaminants from the database.

3.0 Test Cases and Baseline Testing Results

The purpose of the CDBE is to provide users with a means to interact with the chemical database provided with FRAMES. The CDBE should allow users to create a new database, or view/modify contaminant-specific properties in an existing database. The user should also be allowed to add or delete contaminants from the database. In addition to these functions, the CDBE will also provide the function previously provided by the constituent selection glyph in FRAMES for selection of constituents to be included in an analysis.

The following test cases were designed to test that the CDBE meets all of its requirements. As indicated in Table 1 above, a test case may test several requirements. This table can be used to identify which test cases tested each of the requirements.

3.1 Testing Requirement #1, FRAMES Chemical Database Editor

3.1.1 Description and Rationale

Requirement #1: “operate within the FRAMES software system”

This test case verifies the starting of FRAMES, and getting access to the FRAMES Constituent Database Editor (CDBE).

3.1.2 Instructions for Performing the Test and Expected Results

1. Start FRAMES 1.3
2. To start a new case, select New from the File menu. For this test case, type in *File name* box: *CDBE_01.gid*, and select the *Open* button. Enter a Site Name at the prompt and select *Ok*.
3. To begin building the case, double click the *Contaminant* icon, which drops a *black signal light con1* icon into the green worksheet window. (The black signal light indicates that a contaminant database and contaminants have not been selected. Once the database and contaminants are selected, the light will turn green indicating that the module has been completed.)
4. Right click on the black *signal light con1* icon and select from its menu: *General Info*.
5. The *Object General Information* window is displayed. Under *Select from Applicable Models*, select the *FRAMES Default Chemical Database Selection*, then select *OK*
6. Displayed is a *red signal light con1* icon in the green worksheet window.
7. Right click on the *red signal light con1* icon and select from its menu: *User Input*
8. The master database file will open in the *FRAMES Constituent Database Editor* window (*C:\FRAMES\FUI.mdb*), as expected.
9. Select *File, Exit--Discard Changes*

10. Select File, Exit on the main FRAMES screen.
11. Framework--Do you want to save any changes?
12. Select No

3.1.3 Results

The above instructions were followed and the results matched the expectations.

3.2 Testing Requirement #2, FRAMES Chemical Database Editor

3.2.1 Description and Rationale

Requirement #2: “Allow the user to create, access, and save a chemical database”. Note that the ability to create a database is a capability of the CDBE that exists but is not available when the CDBE is invoked through the FRAMES system. The CDBE must be invoked in the stand-alone mode.

3.2.2 Instructions for Performing the Test and Expected Results

Using Windows Explorer, navigate to the FRAMES directory where FRAMES and all of its associated program files are located.

Find the program *Consel.exe* and double click on it. A screen entitled *FRAMES Constituent Database Editor* will appear.

Select *File, NEW Database...*

In the Create FRAMES Database window, and under Select a Database Output Filename, select the Browse button.

In the *Create* window, type in *File name box: CDBE_02iodine.MDB*

Select *Open*

Displayed in the *Create FRAMES Database* window and in the *Select a Database Output Filename* box is: C:\FRAMES\CDBE_02iodine.MDB

Select *Create* button

It displays: *CONTSEL*

Do you want to save changes?

Select *Yes*

Now displayed at the bottom of the *Create FRAMES Database* window is:

Successfully created C:\FRAMES\CDBE_02iodine.MDB

Select *Close* button

Now displayed at the bottom of the *FRAMES Constituent Database Editor* window is *C:\FRAMES\CDBE_02iodine.MDB* (Notice there are no constituents listed in the database at this time).

Select the *Constituent Identification* TAB and enter the following:

Name:	<i>iodine</i>
CAS ID:	<i>11111</i>
Synonyms:	<i>Jodin</i>
Impact: Select:	<i>Chemical, non-carcenogenic inhalation and ingestion</i>
Classification:	<i>Undefined</i>

Select the *Add* button

Select the *Constituent Properties* TAB and enter the following:

Molecular Weight: Value: *125*

Vapor Pressure: Value: *5*

Select *Apply Changes* button

Select the *Constituent of Interest* TAB

Displayed under *Constituents View Options* is:

Group by Impact (radio button was pre-selected)

Select : All Contaminants

Displayed under *Selected Constituents for Analysis* is:

iodine

Jodin

Select *Jodin* and select *Add>>>* to put *Jodin* in the right-hand window (run analysis window)

Select *File, Exit – Save Changes*

Select *File, Exit*

Framework – Do you want to save changes?

Select *Yes*

3.2.3 Results

The above instructions were followed and the results matched the expectations.

3.3 Requirement #3, FRAMES Chemical Database Editor

3.3.1 Description and Rationale

Requirement #3: “Allow the user to select an existing database from a list of available databases (in the FRAMES database format) to be used for an analysis”

3.3.2 Instructions for Performing the Test and Expected Results

Start *FRAMES Contaminant Database* icon on the desktop

The *FRAMES Constituent Database Editor* window, opens.

Select *File*

Select *Open Database...*

It displays the *Open* window with a listing of database files (.mdb)

Select *CDBE_02iodine.mdb*, the database created in the Requirement #2 test case.

Select *Open*

Now it is displaying the *FRAMES Constituent Database Editor* window
(*C:\FRAMES\CDBE_02iodine.mdb*)

Select the *Constituents of Interest* TAB

(You can view constituents by selecting: **Group by Impact** (ordered by name), **Show CAS ID**, or **Group by Classification**, which is expected in Requirement #5)

In the *Select Constituents for Analysis* window, select Jodin
Select *Add>>* to put Jodin in the right-hand window (to run analysis on it)
Select *File, Exit – Save Changes*

3.3.3 Results

The above instructions were followed and the results matched the expectations.

3.4 Requirement #4, FRAMES Chemical Database Editor

3.4.1 Description and Rationale

This test case verifies that the user can select a constituent for viewing or editing.

3.4.2 Instructions for Performing the Test and Expected Results

The test plan, previously developed to test Requirement #3, verified the user could view a constituent and also edit a constituent (iodine was used in that test case).

3.4.3 Results

The above instructions were followed and the results matched the expectations.

3.5 Requirement #5, FRAMES Chemical Database Editor

3.5.1 Description and Rationale

Requirement #5: “Allow the user to select constituents from a list ordered by name or CAS ID”

3.5.2 Instructions for Performing the Test and Expected Results

The testplan previously developed to test Requirement #3 was viewed.

3.5.3 Results

The above instructions were followed and the results matched the expectations.

3.6 Requirement #6, FRAMES Chemical Database Editor

3.6.1 Description and Rationale

Requirement #6: “Allow the user to change any property value associated with constituent”

A printout of the property values was done before and after changing the values; the changes were not saved.

3.6.2 Instructions for Performing the Test and Expected Results

Careful: So you don't corrupt the master database (CDBE.mdb file) while performing this test, do the following steps first:

Copy the CDBE.mdb file to a separate directory on the hard drive.

For this test it is being copied to C:\TESTING\Fui.mdb

Then at C:\TESTING\Fui.mdb, rename the Fui.mdb to: TestCDB.mdb

Then copy the TestCDB.mdb into the C:\FRAMES directory. Now both the master database file (Fui.mdb) and the database file being tested (TestCDB.mdb) are in the C:\FRAMES directory.

Start *FRAMES Contaminant Database* icon on the desktop

The *FRAMES Constituent Database Editor* window, opens.

Select *File*

Select *Open Database...*

It displays the *Open* window with a listing of database files (.mdb)

Then select from the list of files: TestCDB.mdb

Select *Open*

Select the *Constituent of Interest* TAB

Displayed under *Constituents View Options* is:

Group by Impact (radio button was pre-selected)

Select : All Contaminants

Under *Select Constituent for Analysis*, highlight *1,1 dichloroethylene* and

Select *Add>>>* and put *1,1 dichloroethylene* in the right-hand window (run analysis window)

Select the *Constituent Properties* TAB

Do a printout now, before changing the property values

Select *File*

Select *Print...*

Under the *Select Constituents to Print*, highlight *1,1 dichloroethylene*

(Note: the *Print* button is not active until you highlight a constituent to print)

Select *Print* (this gives you a printout of all the property values before changing them)

Select *Close*

Change all the property values

While still having the *Constituent Properties* TAB selected,

enter a property value (or a different property value) for each parameter (based on the range displayed at the bottom of the window). When the property value is within the range, the value turns green, indicating a valid value. Then click on the 'Apply Changes' button.

Example--under Basic Physical Properties category:

CLWM Molecular Weight was: 96.94 changed to: 1

CLVP Vapor Pressure Temperature was: blank changed to: -50

Do a printout now, of property values changed:

Select *File*

Select *Print...*

Under the *Select Constituents to Print*, highlight *1,1 dichloroethylene*

(*Note: the Print button is not active until you highlight a constituent to print*)

Select *Print* (this gives you a printout of all the values after changing them)

Select *Close*

Select *File, Exit – Discard changes*

3.6.3 Results

The above instructions were followed and the results matched the expectations.

3.7 Requirement #7, FRAMES Chemical Database Editor

3.7.1 Description and Rationale

Requirement #7: “Allow the user to *print a paper copy* or *write to a file*, a report of properties for one or more constituents”

3.7.2 Instructions for Performing the Test and Expected Results

The function to allow the user to *print a paper copy* was previously tested when the property values were changed and a printout was done. (see Requirement #6)

3.7.3 Results

The above instructions were followed and the results matched the expectations.

3.8 Requirement #8, FRAMES Chemical Database Editor

3.8.1 Description and Rationale

This requirement has been deleted:

Requirement #8: “Allow the user to create a delimited file of database parameters (e.g. CSV file) for selected constituents and properties”

3.8.2 Instructions for Performing the Test and Expected Results

3.8.3 Results

None. This requirement has been deleted.

3.9 Requirement #9, FRAMES Chemical Database Editor

3.9.1 Description and Rationale

Requirement #9: “Provide help information about the parameters in the database”

3.9.2 Instructions for Performing the Test and Expected Results

Start *FRAMES Contaminant Database* icon on the desktop

The *FRAMES Constituent Database Editor* window, opens.

Use TestCDB.mdb file (not the master Fui.mdb database file)

Select *File*

Select *OPEN Database...*

In the *Open* window, select the *TestCDB.mdb* file

Select *Open* button

Select the *Constituent Properties* TAB

Displayed is:

View: All Contaminants

Name: 1,1 dichloroethylene

Category (jump to): Contaminant Identification

Under the *Basic Physical Properties* category it displays, for example:

<u>Description</u>	<u>Units</u>	<u>Value</u>	<u>Ref</u>
Molecular Weight	g/mol	96.94	327
Water Solubility	mg/L	2250.	282

In the *Description* column, highlight *Molecular Weight*

Select *Help*, then select *How to... F1*

The Help file opens at the parameter for which you requested Help, as expected.

Select *File, Exit* (to close the Help file)

Select *File, Exit--Discard Changes*

3.9.3 Results

The above instructions were followed, and the results matched the expectations.

3.10 Requirement #10, FRAMED Chemical Database Editor

3.10.1 Description and Rationale

Requirement #10: “Provide error messages to the user when inappropriate values are provided for any parameter (as determined by ranges defined within the database)”

3.10.2 Instructions for Performing the Test and Expected Results

Start *FRAMES Contaminant Database* icon on the desktop

The *FRAMES Constituent Database Editor* window, opens.

Use the TestCDB.mdb file (not the master Fui.mdb database file)

Select *File*

Select *Open Database...*

In the *Open* window, select the *TestCDB.mdb* file

Select *Open* button

Select the *Constituents of Interest* TAB

In the *Select Constituents for Analysis* window, highlight *1,1 dichloroethylene*

Select *Add>>* button to put *1,1 dichloroethylene* in the right-hand window (for analysis).

Select the *Constituent Properties* TAB; Displayed is:

View: (Select) Selected Constituents

Name: 1,1 dichloroethylene

Category (jump to): Contaminant Identification

Under the Basic Physical Properties, displayed is (for example):

<u>Description</u>	<u>Units</u>	<u>Value</u>	<u>Ref</u>
Molecular Weight	g/mol	96.94	327

When you select *Molecular Weight*, notice the valid range displayed at the bottom of the window is: (CLWM) Range 1 to 50000.

Select the value of *96.94* (for *Molecular Weight*) and use the backspace key to remove this value. Type in the value of *-1* (which is not within the valid range) and click in a blank space. The *-1* turns pink, indicating an *inappropriate value* was entered, which is the expected result.

Select the *Undo Changes* button

Select *File, Exit—Discard changes*.

3.10.3 Results

The above instructions were followed and the results matched the expectation.

3.1 Requirement # 11, FRAMES Chemical Database Editor

3.11.1 Description and Rationale

Requirement #11: “Operate in Windows 95”. Reworded: Operate in Windows 95/98/NT

3.11.2 Instructions for Performing the Test and Expected Results

The test cases were completed on a Dell OptiPlex GX1p workstation computer, operating in Windows 98 (600MHz, 30GB hard drive, and 256MB RAM).

3.11.3 Results

The above instructions were followed and the results matched the expectations.

3.12 Requirement #12, FRAMES Chemical Database Editor

3.12.1 Description and Rationale

Requirement #12: “Not require modifications to any existing components that run under FRAMES (i.e., GENII and MEPAS).

3.12.2 Instructions for Performing the Test and Expected Results

Outside scope of interactive testing!

3.11.3 Results

Outside scope of interactive testing!

3.13 Requirement #13, FRAMES Chemical Database Editor

3.13.1 Description and Rationale

Requirement #13: “Allow the user to assign references to each property value added or modified”

3.13.2 Instructions for Performing the Test and Expected Results

Start *FRAMES Contaminant Database* icon on the desktop

The *FRAMES Constituent Database Editor* window, opens.

Use the *TestCDB.mdb* file (not the master *Fui.mdb* database file)

Select *File*

Select *Open Database...*

*In the Open window, select the *TestCDB.mdb* file*

Select Open button

Part 1 of test: Add a property value to a constituent and then assign a reference number to it

Select the *Constituents of Interest* TAB

Under the *Select Constituents for Analysis* window, highlight *1,1 dichloroethylene*
Select the *Add>>>* button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Select *Constituent Properties* TAB; displayed is:

View: (Select) *Selected Constituents*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Under the *Basic Physical Properties* category,

Select *Vapor Pressure Temperature* (has no value yet) and type in a value of -50.

Notice that *Vapor Pressure Temperature* has no *Reference number* yet

Highlight the *Vapor Pressure Temperature* Reference cell

Select *References...* from the top menu bar

Select reference number 5 for this test

Select *Apply* (it automatically takes you back to the *Constituents Properties* window)

Select *Apply Changes*

Part 2 of test: *Modify the property value of a constituent and then assign a reference number to it*

While you are still at the *Constituent Properties* TAB, displayed is:

View: (Select) *Selected Constituents*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Under the *Basic Physical Properties* category

Select *Pure contaminant density* for this test, which currently has a *Value = 1*.

Backspace out the 1 and change it to a 20 (it turns green meaning it is within the range)

Notice that currently the *Reference number* for *Pure contaminant density* is currently: 0

Highlight the *Pure contaminant density* Reference cell

Select *References...* (from the top menu)

Select Reference number 1

Select *Apply* button

Notice the Reference number for *Pure contaminant density* is now: 1

Select *Apply Changes*

Select *File, Exit - Discard Changes*

Select *File, Framework-Do you want to save any changes?* No

3.13.3 Results

The above instructions were followed and the results matched the expectations.

3.14 Requirement #14, FRAMES Chemical Database Editor

3.14.1 Description and Rationale

Requirement #14: “Allow the user to *add new references* or select from previous references”

Selecting from a previous reference was already tested in Requirement #13.

3.14.2 Instructions for Performing the Test and Expected Results

Test: To add a new reference

Start *FRAMES Contaminant Database* icon on the desktop
The *FRAMES Constituent Database Editor* window, opens.

Use the TestCDB.mdb file (not the master Fui.mdb database file)

Select *File*

Select *Open Database...*

In the *Open* window, select the *TestCDB.mdb* file

Select *Open* button

Select the *Constituents of Interest* TAB

Under the *Select Constituents for Analysis* window, highlight *1,1 dichloroethylene*

Select *Add>>>* and put *1,1 dichloroethylene* in the right-hand window (run analysis)

Select *Constituent Properties* TAB (note: cannot type a ref number in the grid)

Displayed is:

View: (Select) *Selected Constituents*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Under the *Basic Physical Properties* category,

Select *Pure contaminant density* for this test, which currently has a Ref number of 0 (and a Value of 1)

Select the *Pure contaminant density* Ref cell

Select *References...* from the top menu bar

Select *New* button (it automatically selects the next sequential Reference Number)

Type in the *Short Name* box: This is a new reference number

And type in the *Description* box: This is a new reference being added

Select *Add* button

Select *Apply* (it automatically takes you back to the *Constituents Properties* window)

Select *Apply Changes*

Select *File, Exit-Discard Changes*

3.14.3 Results

The above instructions were followed and the results matched the expectations.

3.15 Requirement #15, FRAMES Chemical Database Editor

3.15.1 Description and Rationale

Requirement #15: “Provide property estimation methods for selected properties (as in the Multimedia-Modeling Environmental Database and Editor (MMEDE)) software”

The testing of Requirement #15 has 17 estimation methods being tested, which are numbered 15.1 through 15.17. The test cases are performed using the TestCDB.mdb file.

Requirement #15	Constituent for Analysis	Property
15.1	1,1 dichloroethylene	Water Solubility, Method S-1, GEMS
15.2	1,1 dichloroethylene	Water Solubility, Method S-2, GEMS
15.3	1,1 dichloroethylene	Water Solubility, Method S-3, GEMS
15.4	1,1 dichloroethylene	Water Solubility, Lyman
15.5	1,1 dichloroethylene	Henry’s Law Constant
15.6	1,1 dichloroethylene	Carbon Matter Partition Coefficient (Koc), GEMS Method, pesticides
15.7	1,1 dichloroethylene	Carbon Matter Partition Coefficient (Koc), GEMS Method, aromatics
15.8	1,1 dichloroethylene	Carbon Matter Partition Coefficient (Koc), Lyman Method, general (various organics)
15.9	1,1 dichloroethylene	Carbon Matter Partition Coefficient (Koc), Lyman Method, aromatics
15.10	1,1 dichloroethylene	Carbon Matter Partition Coefficient (Koc), Lyman Method, s-triazines
15.11	1,1 dichloroethylene	Carbon Matter Partition Coefficient (Koc), Lyman Method, pesticides
15.12	1,1 dichloroethylene	Aqueous Skin Permeability
15.13	1,1 dichloroethylene	Environmental Transfer Factors, Shellfish
15.14	1,1 dichloroethylene	Environmental Transfer Factors, Meat factor
15.15	1,1 dichloroethylene	Environmental Transfer Factors, Milk factor
15.16	1,1 dichloroethylene	Environmental Transfer Factors, Soil to plant transfer factor

Requirement #15	Constituent for Analysis	Property
15.17	1,1 dichloroethylene	Bioaccumulation in Freshwater Fish, Bintein

3.15.2 Instructions for Performing the Test and Expected Results

To verify each of the following estimation methods, the equations in Section 8 of the *DRAFT Requirements for the FRAMES Chemical Database Editor* document will be used. See APPENDIX A for a printout of an Excel spreadsheet used to verify the estimation method calculations.

To verify each of the following estimation methods for selected properties, it is assumed that you are displaying the *FRAMES Constituent Database Editor* window, and that you are ready to select the *Constituents of Interest* TAB. Do exit out of the CDBE between each estimation method tested.

Use the TestCDB.mdb file (not the master Fui.mdb database file)

Select *File*

Select *Open Database...*

In the *Open* window, select the *TestCDB.mdb* file

Select *Open* button

Requirement 15.1 - Testing 1,1 dichloroethylene, Water Solubility, Method S-1

Step A : Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: All Contaminants

Under *Select Constituents for Analysis*,

Select *1,1 dichloroethylene* and use the *Add>>>* button to put *1,1 dichloroethylene* in the right-hand window (run analysis)

Step B: Select the *Constituent Properties* TAB; displayed is:

View: Selected Constituents

Name: 1,1 dichloroethylene

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window is displayed:

Select Property: *Water Solubility*

Input Parameters: (these values should be displayed, or entered if necessary)

Because the estimation method requires a Melting Point, a value must be supplied. In this test, a melting point of -30 is being used, which must be entered.

Octanol Water Partition Coefficient (Kow) = 69.20
Melting Point = -30

Select the following:

Use...	Acid	Based On...
<i>GEMS</i>	grayed out	grayed out

Estimations: (Result)

	Description	Units	Value	Apply
CLSOL	Water Solubility	mg/L	1.53E-01	a

Select the Close button, for testing purposes.

Result: As expected

Instead of exiting out of the CDBE and FRAMES, continue to verify the next estimation method equation.

Requirement 15.2 - Testing 1,1 dichloroethylene, Water Solubility, Method S-2

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: All Contaminants

Under *Select Constituents for Analysis*,

Select *1,1 dichloroethylene* and use the *Add>>>* button to put *1,1 dichloroethylene* in the right-hand window (run analysis)

Step B: Select the *Constituent Properties* TAB; displayed is:

View: Selected Constituents

Name: 1,1 dichloroethylene

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window is displayed:

Select Property: Water Solubility

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 1

Melting Point = -30

Select the following:

Use...	Acid	Based On...
<i>GEMS</i>	grayed out	grayed out

Estimations: (Result)

	Description	Units	Value	Apply
CLSOL	Water Solubility	mg/L	9.99E+00	a

Select the *Close* button, for testing purposes.

Result: As expected

Requirement 15.3 - Testing 1,1 dichloroethylene, Water Solubility

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: All Contaminants

Under Select *Constituents for Analysis*,

Select *1,1 dichloroethylene* and use the *Add>>>* button to put *1,1 dichloroethylene* in the right-hand window (run analysis)

Step B: Select the *Constituent Properties* TAB; displayed is:

View: All Contaminants

Name: 1,1 dichloroethylene

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window is displayed:

Select Property: Water Solubility

Input Parameters: (these values should be displayed, or entered if necessary)

Type in the following, because the equations uses:

Octanol Water Partition Coefficient (Kow) = 69.20

Melting Point = -30

Select the following:

Use... Acid Based On...

***GEMS* a grayed out**

Estimations: (Result)

	Description	Units	Value	Apply
CLSOL	Water Solubility	mg/L	2.38E-01	a

Select the *Close* button, for testing purposes.

Result: As expected

Requirement 15.4, Testing 1,1 dichloroethylene, Water Solubility, Lyman

Step A : Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB; displayed is:

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: *Water Solubility*

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

(No melting point value is used for this Lyman estimation)

Use...	Acid	Based On...
Lyman	grayed out	grayed out

Estimations: (Result)

	Description	Units	Value	Apply
CLSOL	Water Solubility	mg/L	3.07E+02	a

Select *Close* button, for testing purposes.

Result: As expected

Requirement 15.5 - Testing 1,1 dichloroethylene, Henry's Law Constant

Step A : Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is:

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: Henry's Law Constant

Input Parameters: (these values should be displayed, or entered if necessary)

Water Solubility = 2250

Vapor Pressure = 600

Molecular Weight = 96.94

Use... Acid Based On...

Grayed out grayed out grayed out

Estimations: (Result)

	Description	Units	Value	Apply
CLSOL	Henry's Law Constant	atm m ³ /mole	3.40E-02	a

Select the *Close* button, for testing purposes.

Result: As expected

Requirement 15.6 - Testing 1,1 dichloroethylene, Carbon Matter Partition Coefficient (Koc)

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is:

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window is displayed:

Select Property: Carbon Matter Partition Coefficient (Koc)

Input Parameters: (these values should be displayed, or entered if necessary)

Water Solubility = 2250

Use... Acid Based On...

GEMS Method grayed out pesticides

Estimations: (Result)

	Description	Units	Value	Apply
CLKOC	Carbon Matter Partition Coefficient (Koc)	mL/g	6.26E+01	b

Select the *Close* button, for testing purposes.

Result: As expected.

Requirement 15.7- Testing 1,1 dichloroethylene, Carbon Matter Partition Coefficient (Koc)

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is:

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: **Carbon Matter Partition Coefficient (Koc)**

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

<i>Use...</i>	Acid	Based On...
GEMS Method	grayed out	aromatics

Estimations: (Result)

	Description	Units	Value	Apply
CLKOC	Carbon Matter Partition Coefficient (Koc)	mL/g	4.27E+01	a

Select the *Close* button, for testing purposes

Result: As expected.

Requirement 15.8 - Testing 1,1 dichloroethylene, Carbon Matter Partition Coefficient (Koc)

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is:

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: Carbon Matter Partition Coefficient (Koc)

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

Use...	Acid	Based On...
Lyman Method	grayed out	general

Estimations: (Result)

	Description	Units	Value	Apply
CLKOC	Carbon Matter Partition Coefficient (Koc)	mL/g	2.39E+02	a

Select the *Close* button, for testing purposes

Result: As expected.

Requirement 15.9- Testing 1,1 dichloroethylene, Carbon Matter Partition Coefficient (Koc)

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is
 View: *Selected Contaminants*
 Name: *1,1 dichloroethylene*
 Category (jump to): *Contaminant Identification*
 Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:
 Select Property: **Carbon Matter Partition Coefficient (Koc)**
 Input Parameters: (these values should be displayed, or entered if necessary)
 Octanol Water Partition Coefficient (Kow) = 69.20

Use...	Acid	Based On...
Lyman Method	grayed out	aromatics

Estimations: (Result)

	Description	Units	Value	Apply
CLKOC	Carbon Matter Partition Coefficient (Koc)	mL/g	5.23E+01	a

Select the *Close* button (for testing purposes)

Result: As expected.

Requirement 15.10 - Testing 1,1 dichloroethylene, Carbon Matter Partition Coefficient (Koc)

Step A: Select the *Constituents of Interest* TAB
 Under *Constituent View Options*, displayed is:
Group by Impact
 Select: *All Contaminants*
 Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is
 View: *Selected Contaminants*
 Name: *1,1 dichloroethylene*
 Category (jump to): *Contaminant Identification*
 Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:
 Select Property: **Carbon Matter Partition Coefficient (Koc)**

Input Parameters: (these values should be displayed, or entered if necessary)
Octanol Water Partition Coefficient (Kow) = 69.20

<i>Use...</i>	Acid	Based On...
Lyman Method	grayed out	s-triazines

Estimations: (Result)

	Description	Units	Value	Apply
CLKOC	Carbon Matter Partition Coefficient (Koc)	mL/g	5.62E+01	a

Select *Close* button, for testing purposes.

Result: As expected.

Requirement 15.11 - Testing 1,1 dichloroethylene, Carbon Matter Partition Coefficient (Koc)

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the Add>> button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: *The Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: *Carbon Matter Partition Coefficient (Koc)*

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

<i>Use...</i>	Acid	Based On...
Lyman Method	grayed out	pesticides

Estimations: (Result)

	Description	Units	Value	Apply
--	--------------------	--------------	--------------	--------------

CLKOC *Carbon Matter Partition Coefficient
(Koc)* mL/g 5.17E+01 a

Select *Close* button, for testing purposes.

Result: As expected.

Requirement 15.12 - Testing 1,1 dichloroethylene, Aqueous Skin Permeability

Step A : Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the *Add>>* >button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: *Aqueous Skin Permeability*

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

Molecular Weight = 96.94

Use... *Acid* *Based On...*
 grayed out grayed out grayed out

Estimations: (Result)

	Description	Units	Value	Apply
CLKPERM	Aqueous Skin Permeability	cm/hr	9.89E-03	a

Select *Close* button, for testing purposes.

Result: As expected.

Requirement 15.13, 15.14, 15.15, and 15.16 - Testing 1,1 dichloroethylene, Environmental Transfer Factors

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the *Add>>* >button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is

View: Selected Contaminants

Name: 1,1 dichloroethylene

Category (jump to): Contaminant Identification

Select the *Estimate* button

Step C: The window *Estimates for 1,1 dichloroethylene* will be displayed:

Select Property: *Environmental Transfer Factors*

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

***Use...* *Acid* *Based On...*
 grayed out grayed out grayed out**

Estimations: (Results)

	Description	Units	Result Value
15.13, Shellfish:			
CLBFM	Bioaccumulation in Freshwater Mollusk	L/kg	2.30E+00
CLBML	Bioaccumulation in Freshwater Crustacea	L/kg	2.30E+00
15.14, Meat Factor:			
CLFMT	Feed to Animal Meat Transfer Factor	d/kg	1.74E-06
15.15, Milk Factor:			
CLFMK	Feed to Animal Milk Transfer Factor	d/L	5.50E-07
15.16, Soil to plant transfer factor:			
CLBVLV	Soil to Plant Concentration Ratio for Leafy Vegetables	kg/kg	3.35E+00
CLBVRV	Soil to Plant Concentration Ratio for Root Vegetables	kg/kg	3.35E+00
CLBVOV	Soil to Plant Concentration Ratio, Other Vegetables	L/kg	3.35E+00
CLBVFR	Soil to Plant Concentration Ratio for Fruit	kg/kg	3.35E+00
CLBVCL	Soil to Plant Concentration Ratio for Cereal	kg/kg	3.35E+00
CLBVAF	Soil to Plant Concentration Ratio for Animal Forage	kg/kg	3.35E+00
CLBVAH	Soil to Plant Concentration Ratio for Hay	kg/kg	3.35E+00
CLBVAG	Soil to Plant Concentration Ratio for Grain	kg/kg	3.35E+00

Select *Close* button, for testing purposes.

Result: As expected.

15.17 - Testing 1,1 dichloroethylene, Bioaccumulation In Freshwater Fish

Step A: Select the *Constituents of Interest* TAB

Under *Constituent View Options*, displayed is:

Group by Impact

Select: *All Contaminants*

Select *1,1 dichloroethylene* and use the *Add>>* >button to put *1,1 dichloroethylene* in the right-hand window (for analysis)

Step B: Select the *Constituent Properties* TAB, displayed is

View: *Selected Contaminants*

Name: *1,1 dichloroethylene*

Category (jump to): *Contaminant Identification*

Select the *Estimate* button

Step C: The *Estimates for 1,1 dichloroethylene* window will be displayed:

Select Property: *Bioaccumulation in Freshwater Fish*

Input Parameters: (these values should be displayed, or entered if necessary)

Octanol Water Partition Coefficient (Kow) = 69.20

<i>Use...</i>	<i>Acid</i>	<i>Based On...</i>
Bintein	grayed out	grayed out

Estimations: (Result)

	Description	Units	Value	Apply
CLBFF	Bioaccumulation in Freshwater Fish	L/kg	7.73E+00	a

Select *Close* button, for testing purposes.

Result: As expected.

3.16 Requirement #16, FRAMES Chemical Database Editor

3.16.1 Description and Rationale

Requirement #16: “Allow the user to select or deselect constituents to be included in an analysis”

3.16.2 Instructions for Performing the Test and Expected Results

The testing of Requirement #3 verified the user could select (Add>>>) or deselect (<<<Remove) constituents to be included in an analysis.

3.16.3 Results

The above instructions were followed and the results matched the expectations.

3.17 Testing Requirement #17, FRAMES Chemical Database Editor

3.17.1 Description and Rationale

Requirement #17: “Allow the user to view constituents grouped by chemical groups (e.g., polycyclic aromatic hydrocarbons)”

3.17.2 Instructions for Performing the Test and Expected Results

Start *FRAMES 1.3*

To start a new case, select **New** from the **File** menu. For this test case, type in *File name* box: *CDBE_17.gid*, and select the *Open* button. Enter a Site Name at the prompt and select **Ok**.

To begin building the case, double click the *Contaminant* icon, which drops a *black signal light con1* icon into the green worksheet window.

Right click on the *black signal light con1* icon and select from its menu: *General Info*.

The *Object General Information* window is displayed. Under *Select from Applicable Models*, select the *FRAMES Default Chemical Database Selection*, then select **OK**.

Displayed is a *red signal light con1* icon in the green worksheet window.

Right click on the *red signal light con1* icon and select from its menu: *User Input*

Now it is displaying the *FRAMES Constituent Database Editor* window.

The *Constituents of Interest* TAB is displayed. Select the radio button:

- *Group by Classification*

Select:

nitriles u (7)

Select Constituents for Analysis

Add>>>

<<<Remove

Acetonitrile
Acrylonitrile
Isopropene cyanide
methyl cyanide
Methylacrilonitrile
Propenenitrile
Vinyl cyanide

Select *File* , *Exit-Discard Changes*

Select *File*, *Exit*

Framework - Do you want to save any changes? Select No

3.17.3 Results

The above instructions were followed and the results matched the expectations

3.18 Testing Requirement #18, FRAMES Chemical Database Editor

3.18.1 Description and Rationale

Requirement #18: “The user should also be allowed to add or delete contaminants from the database”

3.18.2 Instructions for Performing the Test and Expected Results

Deleting a contaminant from a database,

Start *FRAMES Contaminant Database* icon on the desktop

The *FRAMES Constituent Database Editor* window, opens.

(Do not use the master Fui.mdb database file)

NOTE: The database (Requirement18.MDB) is being used only for the purpose to test the ability to delete and to add a contaminant to this specific database. The Requirement18.mdb file is a copy of the Fui.mdb file that was renamed.

Select *File, Open Database...*

Select *Requirement18.MDB*

Select *Open*

Select the *Constituents of Interest* TAB

Select *1,1 dichloroethylene* and use the *Add>>* button to put *1,1 dichloroethylene* in the right-hand window (for analysis).

Select the *Constituent Identification* TAB

Select the *Delete* button. It displays:

Delete Constituent:

“Are you sure you want to delete all data for: 1,1 DICHLOROETHYLENE (75354)”

YES

NO

Select *Yes*

Select *File, Exit - Save Changes*

ERROR: (Con1)

Error reported by C:\FRAMES\cont.exe Fui.mdb

“Error for Constituent Database” No contaminants selected for simulation!”

This error message is expected because you deleted a selected contaminant in the database. You'll notice that the contaminant was actually deleted from the database.

Select *File, Exit*

Adding a contaminant to a database,

Start *FRAMES Contaminant Database* icon on the desktop
The *FRAMES Constituent Database Editor* window, opens.

NOTE: The database (Requirement18.MDB) is being used only for the purpose to test the ability to delete and to add a contaminant to this specific database.

Select *File, Open Database...*

Select *Requiremen18.MDB*

Select *Open*

Select the *Constituent of Interest* TAB

NOTE: Must do this step (or you will get an error message upon exiting FRAMES that no contaminant was selected):

Select *1,1 dichloroethylene* and use the *Add>>>* button to put *1,1 dichloroethylene* in the right-hand window (for analysis).

Select the *Constituent Identification* TAB

View: *All Contaminants*

Name: type in: *1,1 testing add a contaminant*

CASID: type in: *121212*

Synonyms: type in: *none*

Impact: leave as: *Chemical, carcinogenic inhalation and ingestion*

Classification: leave as: *Undefined*

Select the *Add* button

Select *File, Exit - Save Changes*

Go back to the *Constituent of Interest* TAB and notice that the new contaminant is now on the list.

Select *File, Exit - Save Changes*

3.18.3 Results

The above instructions were followed and results were as expected

APPENDIX ACDBE Estimation Methods

This is a printout of an Excel spreadsheet (CDBE_est_test.xls) used to verify the estimation methods calculations, CDBE Requirement #15.

1,1 dichloroethylene

Water Solubility, See TAB: WaterSol in the Excel file: CDBE_est_test.xls

Method S-1 Requirement 15.1

Kow 69.2

Log Kow 1.840106094 $\text{Log S} = -1.1123 \text{ Log Kow} + 0.686 - 0.0099 \text{ (mp-25)}$

Melting Point-30

Log S -0.816250009

S 0.152668694

Code 1.53E-01 OK

Method S-2 Requirement 15.2

Kow 1 Temporary change

Log Kow 0

Melting Point-30 $\text{Log S} = -1.034 \text{ log Kow} + 0.455 - 0.0099 \text{ (mp-25)}$

Log S 0.9995

S 9.988493699

Code 9.99E+00 OK

Method S-3 Requirement 15.3

Kow 69.2

Log Kow 1.840106094 $\text{Log S} = -0.65 \text{ log Kow} + 0.0279 - 0.0099 \text{ (mp-25)}$

Melting Point-30

Log S -0.623668961

S 0.237865271

Code 2.38E-01 OK

Lyman Requirement 15.4

Kow 69.2

Log Kow 1.840106094 $\text{Log S} = -0.922 \text{ log Kow} + 4.184$

Log S 2.487422181

S 307.2006858

Code 3.07E+02

1,1 dichloroethylene

Requirement 15.5

Henry's Law Constant, See TAB: HLC in the Excel file: CDBE_est_test.xls
VaporPressure/Solubility Method

vap 600
mw 96.94 HLC = (vap mw) / (760 S)
WS 2.25E+03 mg/L
HLC 3.40E-02
Code 3.40E-02 OK

1,1 dichloroethylene

Carbon Matter Partition Coefficient (Koc),

See TAB: KOC in the Excel file: CDBE_est_test.xls

GEMS: Pesticides, based on solubility Requirement 15.6

WS 2.25E+03
log WS 3.352182518 log Koc = -0.55 log S + 3.64
Log Koc 1.80E+00
Koc 6.26E+01
Code 6.26E+01 OK

GEMS: Aromatics, based on Kow Requirement 15.7

Kow 6.92E+01
log Kow 1.840106094 Log Koc = log Kow - 0.21
Log Koc 1.63E+00
Koc 4.27E+01
Code 4.27E+01 OK

Lyman: Various organics Kow 0.001 and 4E6 Requirement 15.8

Kow 6.92E+01 (uses "general" chemical class)
log Kow 1.840106094 log Koc = 0.544 log Kow + 1.377
Log Koc 2.38E+00
Koc 2.39E+02
Code 2.39E+02 OK

Lyman: Aromatics Kow 100 and 4E6 Requirement 15.9

Kow 6.92E+01
log Kow 1.840106094 log Koc = 0.937 log Kow - 0.006
Log Koc 1.72E+00
Koc 5.23E+01
Code 5.23E+01 OK

Lyman: s-triazines Requirement 15.10

Kow 6.92E+01
log Kow 1.840106094 log Koc = 0.94 log Kow + 0.02

Log Koc 1.75E+00
Koc 5.62E+01
Code 5.62E+01 OK

Lyman: Pesticides Requirement 15.11
Kow 6.92E+01
log Kow 1.840106094 $\log Koc = 1.029 \log Kow - 0.18$
Log Koc 1.71E+00
Koc 5.17E+01
Code 5.17E+01 OK

1,1 dichloroethylene Requirement 15.12
Aqueous Skin Permeability, See TAB: SkinPerm in the Excel file: CDBE_est_test.xls
EPA Dermal Handbook method
Kow 69.2
mw 96.94 $\log Kp = -2.72 + 0.71 \log Kow - 0.0061$
Log Kow 1.84E+00
Log Kp -2.00E+00
Kp 9.89E-03
Code 9.89E-03 OK

1,1 dichloroethylene
Environmental Transfer Factors,
See TAB: ETFs in the Excel file: CDBE_est_test.xls
Shellfish Requirement 15.13
Kow 69.2
Log Kow 1.84E+00 $\log BCS = 0.819 \log Kow - 1.146$
log BCS 3.61E-01
BCS 2.30E+00
Code 2.30E+00 OK Used also for Mollusk

Meat factor Requirement 15.14
Kow 69.2
Log Kow 1.84E+00 $\log FMT = -7.6 + \log Kow$
Log FMT -5.76E+00
MFT 1.74E-06
Code 1.74E-06 OK

Milk factor Requirement 15.15
Kow 69.2
Log Kow 1.84E+00 $\log FMK = -8.1 + \log Kow$
Log FMK -6.26E+00
FMK 5.50E-07
Code 5.50E-07 OK

Soil to plant transfer factor Requirement 15.16

Kow 69.2 Note: CR = STP

Log Kow 1.840106094

Log CR 5.24E-01 log CR = 1.588 - 5.78 log Kow Dry Weight

CR 3.35E+00 Dry Weight

1,1 dichloroethylene

Bioaccumulation in Fish, See TAB: BCFish in the Excel file: CDBE_est_test.xls)

Devillers, Bintein and Domine Requirement 15.17

Kow 69.2 log BCF = 0.76 log Kow - 0.23

mw 96.94

Log Kow 1.84E+00

log BCF 8.88E-01

BCF 7.73E+00

Code 7.73E+00 OK