



## Computed T1MX in NMRD Profile Wizard: Problems, solutions and a discussion of merits

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### Introduction

A previous Application Note (AN040913) has described the way one can modify the default behavior and capabilities of AcqNmr parameters with respect to expressions and parameter formulae. For illustration purposes, we have used an example when one would like to define T1MX as a function of the relaxation field BRLX.

In this Note, we shall consider this special case on its own merit.

While the required modification for single, manually controlled experiments is quite easy and straightforward, the idea of computed T1MX clashes with the philosophy of the current Profile Wizard (versions **up to 2.1.0.55**). This may be revised in one of the future versions but, at this moment, we have to live with it.

Trying to implement computed T1MX within the Wizard presents two problems:

--- First of all, the values of the acquisition parameters listed in the Wizard are intended exclusively as numeric constant. For example, setting the Wizard's T1MX edit box to  $(0.3/(1+BRLX*BRLX))$  and pressing Execute, the input string is converted to 0 because of its inherently illegal syntax.

--- Second problem consists in the fact that the option "Before each point, estimate T1MX" is no longer pertinent since T1MX, being computed, should not be estimated from experimental data. Any estimate of T1MX in fact implies setting its numeric value which overrides any previous definition by means of an expression (this is a reason why the old macro Profile also can not be used).

### A simple solution

In this Note we describe a simple solution for overcoming the above problems. The idea is to redefine the FFC acquisition sequences making them use a parameter such as AUX1 in place of T1MX. The value of AUX1 can be defined by means of a formula involving BRLX which the Wizard shall never change. On the other hand, whatever the Profile Wizard does with the T1MX parameter is of no consequence since it has no effect on the pulse sequence.

We shall now describe the distinct steps which need to be done.

**Step 1:** Making BRLX a legal name for an expression variable.

As described in the Application Note AN040913, this requires a modification of the plain text DefaultParameters.def file, replacing the line

```
BRLX|Relaxation field |6| 3| 17|ADWUF |.1 |R |0,1000 |
```

with

```
BRLX|Relaxation field |6| 3| 17|ADWUFVp |.1 |R |0,1000 |
```

(note : trailing comment sections are not shown and modifications are marked in bold red text).

It is not necessary to modify the definition of T1MX since we shall not use it.

**Step 2:** Modifying the FFC NMR sequences you intend to use in order to make them use the parameter AUX1 in place of T1MX. In what follows, we shall assume that the desired sequences are the usual PP/S and NP/S.

Make a copy of the file *DefaultFfcSequences.ssf* and rename it as, say, *AUX1\_FfcSequences.ssf*.

Now, using a plain text Editor, locate the scripts for the two sequences and, within each section, replace all occurrences of T1MX with AUX1. The modified scripts shall look like this (modifications are marked in bold red face and comment lines are stripped for the sake of brevity):

**SEQUENCE PP/S**

```

D0;D1;D2;D3;D4;D5;D6;PW;RINH;ACQD;STIM
#SETUP
D0 :(RD) [m(O)] 'Recycle delay
D1 :(4*AUX1-TAU)[m(R)] 'Balancing
D2 =(SWT) [m(P)] 'Switching to pol.field
D3 :(TPOL)[m(P)] 'Polarization
D4 =(SWT) [m(R)] 'Switching to rlx.field
D5 :(TAU) [m(R)] 'Relaxation interval tau
D6 =(SWT) [m(A)] 'Switching to acq.field
PW = 90 [m(A) p(x,-x,y,-y)]
RINH [m(A)]
ACQD [m(A)]
STIM [m(A)]
ENDS [m(O) p(x,-x,y,-y)] 'Accumulation
'-----
TPOL=.1
BRLX 0.1
'-----
NBLK= 1          'Multi-blocks
BACR= "TAU"
BINI= (4*AUX1)
NBLK= 16
END SEQUENCE

```

**SEQUENCE NP/S**

```

D0;D1;D2;D3;D4;D5;D6;PW;RINH;ACQD;STIM
#SETUP
D0 :(RD) [m(O)] 'Recycle delay
D1 =(4*AUX1-TAU) [m(R)] 'Balancing
D2 =(SWT) [m(O)] 'Switching to zero field
D3 :(4*AUX1)[m(O)] 'Zero field interval
D4 =(SWT) [m(R)] 'Switching to rlx.field
D5 :(TAU) [m(R)] 'Magnetization build-up
D6 =(SWT) [m(A)] 'Switching to acq.field
PW =90[m(A) p(x,-x,y,-y)]
RINH [m(A)]
ACQD [m(A)]
STIM [m(A)]
ENDS [m(O) p(x,-x,y,-y)] 'Accumulation
'-----
BRLX 4
'-----
NBLK= 1          'Multi-blocks
BACR= "TAU"
BINI= (4*AUX1)
NBLK= 16
END SEQUENCE

```

**Hint:** If you wish, you can efficiently and modify all sequences in the AUX1\_FfcSequences.ssf file by replacing **all** occurrences of T1MX with AUX1.

**Step 3:** Run AcqNmr and set into AUX1 (located in the *AcqPar\User* parameters page) the desired formula, such as

$$AUX1 = (0.3/(1+BRLX*BRLX))$$

**Hint:** If you wish to increase the persistence of the setting, making it a default for the modified sequence, insert the above line into the SETUP sections of the sequences scripts (for example, just before the END

SEQUENCE lines). In this case, Step 3 becomes unnecessary. It also makes it easier to edit the formula off-line when it becomes complicated.

**Step 4 (optional):** Load one of the desired sequences from the AUX1\_FfcSequences.ssf file. You can now verify in the Immediate Mode that it really works as intended.

**Step 5:** Run the Profile Wizard dialog.

Make sure that you load the high- and low-field sequences from the file AUX1\_FfcSequences.ssf.

The option "*Repeat point if TIMX was off tolerance*" should be unchecked (though it is not particularly harmful and might even be still of some use).

All other options still maintain their usual meaning.

The starting value of TIMX is nearly irrelevant. Only in the case when any of the TIMX-related options is checked, the best choice is the value obtained from the AUX1 formula for the starting BRLX value (it may help to avoid an unnecessary repetition of the first measurement).

**Step 6:** Execute the Wizard.

The Wizard will do all its tricks but it will not affect the timing of the acquisition sequence, not even when it is allowed to change the value of TIMX (for example, during the preliminary setup or when the option "*Before each point, estimate TIMX*" is checked).

### Conclusion and discussion of merits

The modifications described in this Note respond to a specific request from the field and are linked to the measurements of systems with a wide distribution of relaxation rates (strongly non-exponential relaxation decay curves). In these case, one often needs to measure the decay curves very carefully (long acquisition times), using a large number of logarithmically distributed blocks (e.g., NBLK=128) and a rather large number of scans.

In such samples the AcqNmr mono-exponential fits used for estimating a suitable TIMX are not quite adequate and the proper TIMX setting should be considerably greater than the 'mono-exponential' TIMX in order to avoid distortions of the relaxation decays of components with the longest  $T_1$ 's.

While the approach outlined this Note may be an answer (at least in certain situations), the Author is not really convinced that this is the best road to follow. In fact, after having measured many tens of poly-disperse systems, I have yet to encounter a sample which could not be adequately measured in one of the following ways:

(1) In a great majority of cases (such as in rocks and other porous samples) the components with the longest  $T_1$ 's correspond to bulk water (or other solvent) and have almost negligible field-dependence. In such cases, it is *necessary* to set TIMX to a fixed value (e.g., 2.5 s) and tell the Profile Wizard not to change it, unchecking the options "*Before each point, estimate TIMX*" and "*Repeat point if TIMX was off tolerance*".

(2) In many cases it is possible to get very decent automatic estimates of the longest  $T_1$ 's by setting the evaluation parameters BINI (initial block) and BEND (final block) to the trailing portion of the relaxation decay curve. In Author's experience, for example, when 128 TAU values are used and distributed logarithmically from 0.001 to 2.5 s, the choice of BINI=1 and BEND=64 leads to a *very good estimate of the longest  $T_1$ 's* present in the sample. With these settings, it is then perfectly plausible to use standard sequences and standard Profile Wizard.

These critical remarks, however, do not mean that the approach described in this Note is not a valid alternative and that it might not turn useful in special cases. In any case, the Note provides the technicalities of its implementation within the current software.