Structure for specifying the model

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1 Current Structure

I will need to go through more examples but I see the current structure as

```
> AE1 <-
+     list(PFIMmodel=function(tim, parModel, parArms, model)
+      {
+          V <- parModel[1]
+          k <- parModel[2]
+          Alin <- parModel[3]
+          dose <- parArms[1]
+          nDoses <- parArms[2]
+
+          PK <- 0
+          for (idx in 0:(nDoses-1)) {
+              PK <- PK + (tim>=idx*24)*dose/V*(exp(-k*(tim-idx*24)))
+          }
+          PD <- Alin*PK
+
+          cbind(PK,PD)
+      },
+          Type='AE',
+          parModelName=c('V','k','Alin'),
+          parModel=c(4.5,0.5,3),
+          parModelVar=c(0.2,0.4,0.15),
+          parModelVarType='exp',
+          parObsName=c('Conc','Effect'),
+          parObsErr=list(c(0.3,0.5), c(0,0.3)),
+          parObsTimes=
+          list(list(c(0.5,1,2,4,8,12,24,48),
+                    c(0,4,8,12,24,48)),
+               list(c(0.5,1,2,4,8,12,24),
+                    c(0,4,8,12,24)),
+               list(c(0.5,1,4,12,23.9,47.9,71.9),
+                    c(0,4,12,23.9,47.9,71.9))),
+          parArmsName=c('dose','nDoses'),
```

```
+          parArms=list(c(100,30,5), c(1,1,3)),
+          ArmsName=list('100 mg','30 mg','10 mg'),
+          TimeName='Time (hr)',
+          tRange=c(0,72),
+          mpOpt=list()
+          )
```

2 Proposed Changes

I would change the model parameters to a numeric matrix with named rows (or columns, whichever made more sense). For rows it would look like

```
> (parModel <- matrix(c(4.5, 0.5, 3, 0.2, 0.4, 0.15), ncol=2L,
+                     dimnames=list(c('V','k','Alin'), c('val', 'var'))))
```

```
     val  var
V    4.5 0.20
k    0.5 0.40
Alin 3.0 0.15
```

You obtain the values and the variances as named vectors by extracting the column and specifying `drop` to be `TRUE`.

```
> parModel[, 'val', drop=TRUE]
```

```
   V    k Alin
 4.5  0.5  3.0
```

Alternatively, the model parameters could be specified as a data frame with row names.

```
> (parModel <- data.frame(value=c(4.5,0.5,3), variance=c(0.2,0.4,0.15),
+                         row.names=c('V','k','Alin')))
```

```
     value variance
V      4.5     0.20
k      0.5     0.40
Alin   3.0     0.15
```

Then it is even easier to extract the values and the variances except that you need to assign the names separately.

```
> pars <- parModel$value
> names(pars) <- row.names(parModel)
> pars
```

```
   V    k Alin
 4.5  0.5  3.0
```

A middle ground is to use the data.frame structure and convert it to a matrix before extracting

```
> data.matrix(parModel)[, 'value', drop=TRUE]
```

```
   V    k Alin
 4.5  0.5  3.0
```

The observation error structure could be a named list or another matrix or a data frame. Probably

```
> (parObsErr <- data.frame(Conc=c(0.3,0.5), Effect=c(0,0.3)))
```

```
  Conc Effect
1  0.3    0.0
2  0.5    0.3
```

The arms specification could be another data frame

```
> (Arms <- data.frame(dose=c(100,30,5), nDoses=c(1,1,3),
+                     row.names=c('100 mg','30 mg','10 mg')))
```

```
       dose nDoses
100 mg  100      1
30 mg    30      1
10 mg     5      3
```

(By the way, I got this example from the file `model.defaultAEfun.R` and either the last name or the last dose is incorrect.

3 Summary

So I would change the model specification to

```
> AE1 <-
+     list(PFIMmodel=function(tim, parModel, parArms, model)
+      {
+          V <- parModel[1]
+          k <- parModel[2]
+          Alin <- parModel[3]
+          dose <- parArms[1]
+          nDoses <- parArms[2]
+
+          PK <- 0
+          for (idx in 0:(nDoses-1)) {
+              PK <- PK + (tim>=idx*24)*dose/V*(exp(-k*(tim-idx*24)))
+          }
+          PD <- Alin*PK
+
+          cbind(PK,PD)
```

```
+      },
+          Type='AE',
+          parModel=data.frame(value=c(4.5,0.5,3),
+                              variance=c(0.2,0.4,0.15),
+                              row.names=c('V','k','Alin')),
+          parModelVarType='exp',
+          parObsErr=data.frame(Conc=c(0.3,0.5),
+                               Effect=c(0,0.3)),
+          Arms=data.frame(dose=c(100,30,5), nDoses=c(1,1,3),
+                          row.names=c('100 mg','30 mg','10 mg')),
+          parObsTimes=
+          list(list(c(0.5,1,2,4,8,12,24,48),
+                    c(0,4,8,12,24,48)),
+               list(c(0.5,1,2,4,8,12,24),
+                    c(0,4,8,12,24)),
+               list(c(0.5,1,4,12,23.9,47.9,71.9),
+                    c(0,4,12,23.9,47.9,71.9))),
+          TimeName='Time (hr)',
+          tRange=c(0,72),
+          mpOpt=list()
+          )
```

I will look at other examples. In the meantime, do either of you have comments?