

RLumModel - Fitting model parameters to experimental data

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Introduction

Preparing

```
parRanges <- data.frame(min = c(5.1e7, 1e5, 1e9, 2.5e6, 5e8, 3e6, 1e8, 1e6, 5e7),
                        max = c(5.1e11, 1e9, 1e13, 2.5e10, 5e12, 3e10, 1e12, 1e10, 5e11))

rownames(parRanges) <- c("N1", "N2", "N3", "N4", "N5", "N6", "N7", "N8", "N9")

sequence <- list(
  TL = c(20, 450, 5),
  IRR = c(20, 5, 0.5),
  TL = c(0, 450, 5))

model <- "Pagonis2007"

func_FME <- fit_data2RLumModel(
  sequence = sequence,
  model = model,
  seq.step2fit = 3)

parms <- extract_pars2FME(model = model)
```

Data fitting for TL data

```
global_Sens <- FME::sensRange(func = func_FME,
                              parms = parms,
                              dist = "latin",
                              sensvar = c("signal"),
```

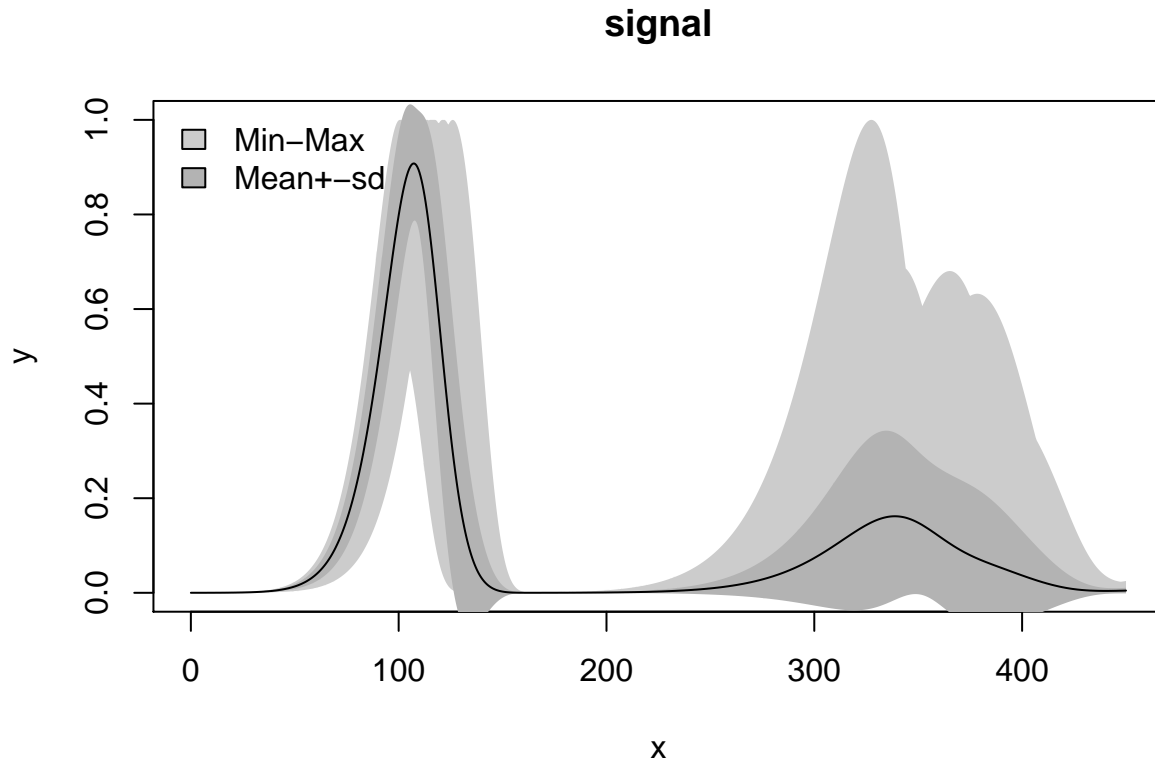
```

      parRange = parRanges,
      num = 50
    )

global_Sens_sum <- summary(global_Sens)

plot(global_Sens_sum)

```



```

SensR <- FME::sensFun(func = func_FME,
  parms = parms,
  sensvar = c("signal"),
  senspar = c("N1", "N2", "N3", "s1", "s2", "s3", "E1", "E2", "E3")
)

summary(SensR)

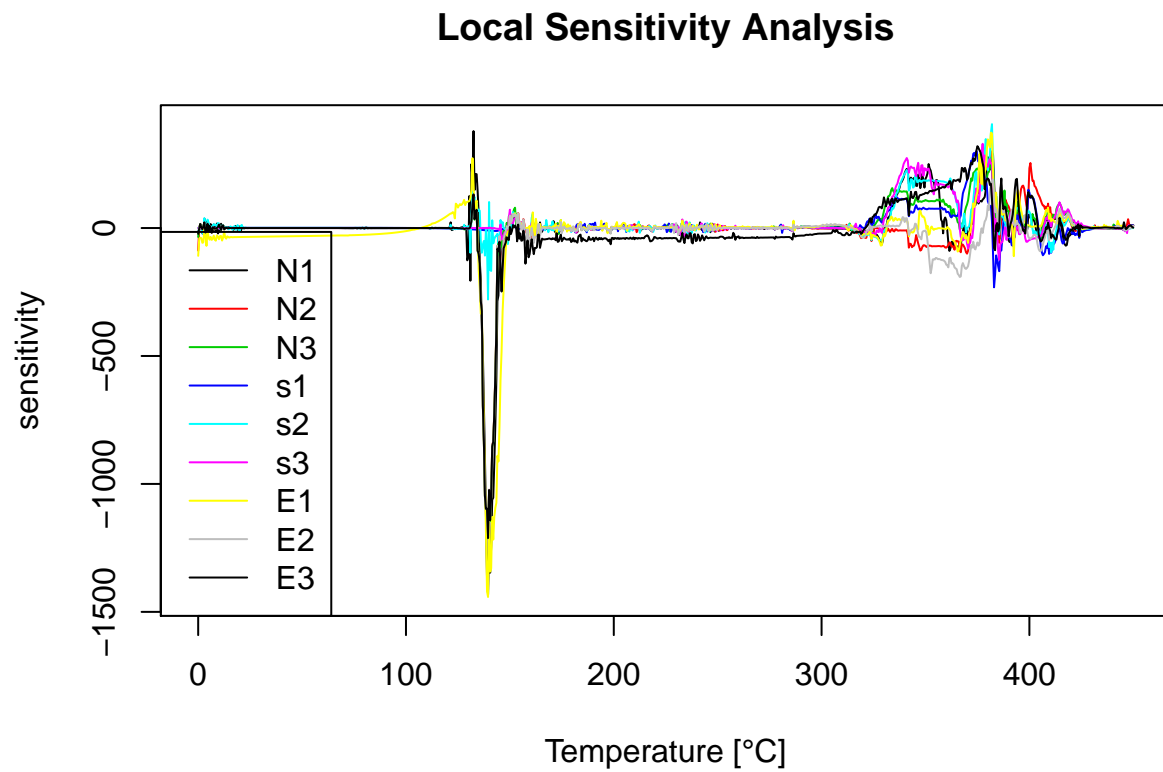
```

```

##      value  scale L1  L2  Mean   Min Max   N
## N1 5.1e+09 5.1e+09 42 4.8  -3.5 -1432 379 901
## N2 1.0e+07 1.0e+07 36 4.2  -9.6 -1210 304 901
## N3 1.0e+11 1.0e+11 37 4.2   3.7 -1214 274 901
## s1 5.0e+12 5.0e+12 22 1.7  11.1  -232 301 901
## s2 5.0e+14 5.0e+14 28 2.1  18.6  -279 406 901
## s3 3.6e+14 3.6e+14 26 2.1  18.6  -124 329 901
## E1 9.7e-01 9.7e-01 49 5.4 -17.8 -1442 373 901
## E2 1.6e+00 1.6e+00 32 4.1 -20.1 -1210 189 901
## E3 1.7e+00 1.7e+00 56 4.5  -7.4 -1212 320 901

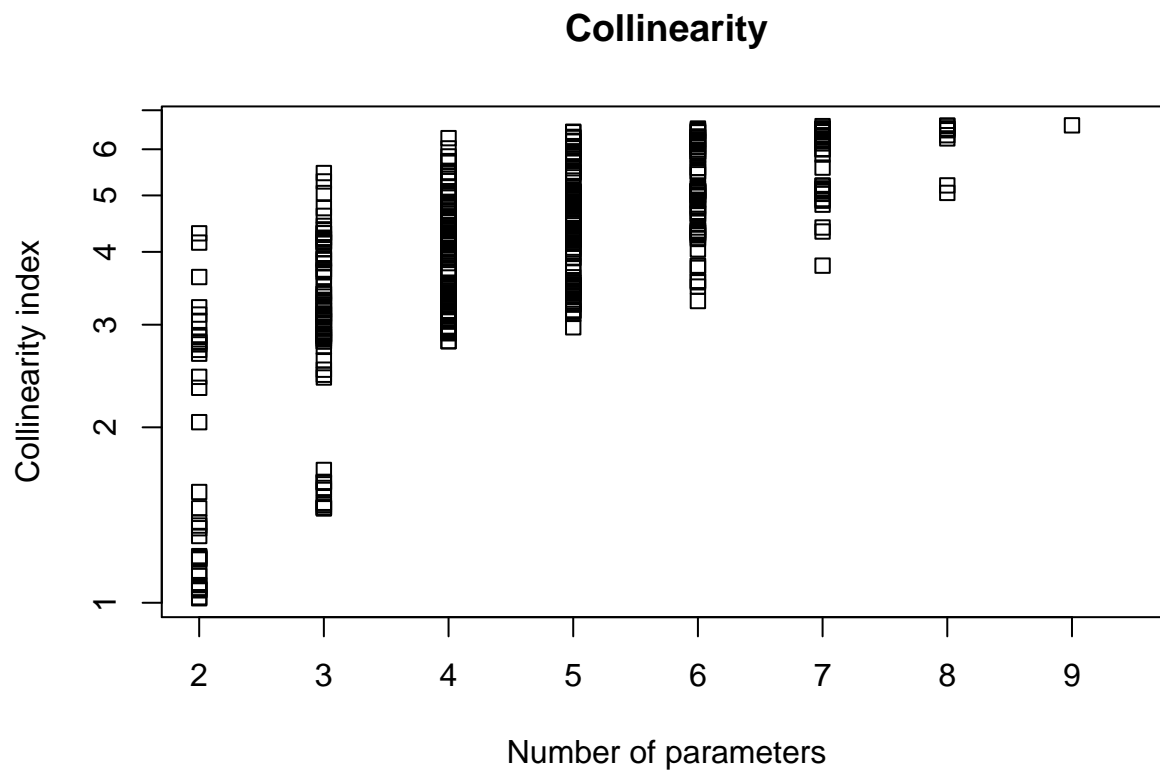
```

```
plot(SensR, legpos = "bottomleft", xlab = "Temperature [\u00B0C]", main = "Local Sensitivity Analysis")
```



```
Coll <- FME::collin(SensR)
```

```
plot(Coll, log = "y")
```



```
data("ExampleData.FittingTL")
exp_data <- get_RLum(TL_fitting_data, record.id = 2)
exp_data <- get_RLum(exp_data)
exp_data[,2] <- exp_data[,2]/max(exp_data[,2])
colnames(exp_data) <- c("time", "signal")
```

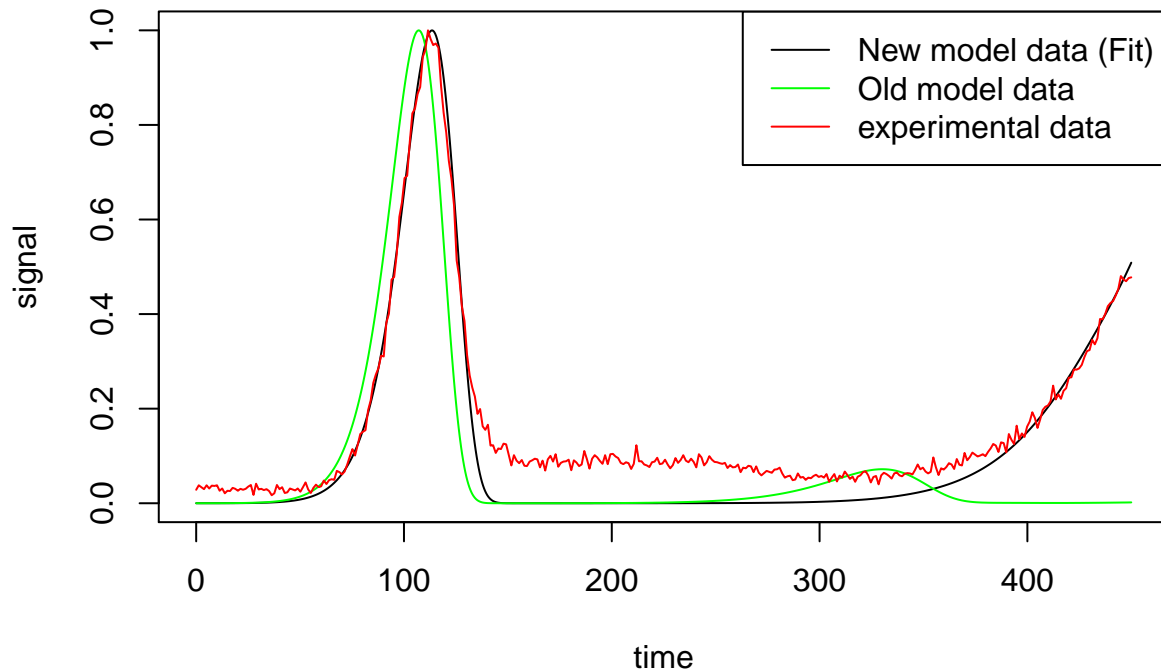
```
Fit_func <- function(x, parset = names(x)){
  parms[parset] <- exp(x)
  out <- func_FME(parms)
  return(modCost(model = out, obs = exp_data))
}
```

```
Fit_TL <- modFit(f = Fit_func,
  p = log(c(parms[parms != 0])),
  method = "Port")
```

| ## | | old | new | percent |
|----|----|----------|--------------|-----------|
| ## | N1 | 5.10e+09 | 5.071618e+09 | 99.44349 |
| ## | N2 | 1.00e+07 | 1.005292e+07 | 100.52917 |
| ## | N3 | 1.00e+11 | 1.026715e+11 | 102.67153 |
| ## | N4 | 2.50e+08 | 2.537518e+08 | 101.50072 |
| ## | N5 | 5.00e+10 | 4.844584e+10 | 96.89168 |
| ## | N6 | 3.00e+08 | 3.064441e+08 | 102.14802 |
| ## | N7 | 1.00e+10 | 9.961810e+09 | 99.61810 |
| ## | N8 | 1.00e+08 | 1.008282e+08 | 100.82820 |
| ## | N9 | 5.00e+09 | 4.990810e+09 | 99.81620 |

| | | | |
|----------|----------|--------------|-----------|
| ## E1 | 9.70e-01 | 9.886116e-01 | 101.91872 |
| ## E2 | 1.55e+00 | 1.563571e+00 | 100.87558 |
| ## E3 | 1.73e+00 | 1.963930e+00 | 113.52195 |
| ## E4 | 1.80e+00 | 1.805885e+00 | 100.32695 |
| ## E5 | 2.00e+00 | 1.656122e+00 | 82.80611 |
| ## E6 | 1.43e+00 | 1.431264e+00 | 100.08838 |
| ## E7 | 1.75e+00 | 1.605608e+00 | 91.74905 |
| ## E8 | 5.00e+00 | 5.000000e+00 | 100.00000 |
| ## E9 | 5.00e+00 | 5.000000e+00 | 100.00000 |
| ## s1 | 5.00e+12 | 5.010717e+12 | 100.21435 |
| ## s2 | 5.00e+14 | 5.005148e+14 | 100.10296 |
| ## s3 | 3.60e+14 | 3.625869e+14 | 100.71859 |
| ## s4 | 1.50e+13 | 1.487645e+13 | 99.17636 |
| ## s5 | 1.00e+10 | 1.024899e+10 | 102.48995 |
| ## s6 | 5.00e+13 | 5.004402e+13 | 100.08804 |
| ## s7 | 5.00e+14 | 4.934574e+14 | 98.69148 |
| ## s8 | 1.00e+13 | 1.000000e+13 | 100.00000 |
| ## s9 | 1.00e+13 | 1.000000e+13 | 100.00000 |
| ## A1 | 1.00e-08 | 9.822049e-09 | 98.22049 |
| ## A2 | 1.00e-09 | 1.005724e-09 | 100.57242 |
| ## A3 | 5.00e-10 | 5.215049e-10 | 104.30098 |
| ## A4 | 5.00e-10 | 4.981714e-10 | 99.63428 |
| ## A5 | 1.00e-10 | 9.780327e-11 | 97.80327 |
| ## A6 | 5.00e-07 | 5.063437e-07 | 101.26873 |
| ## A7 | 1.00e-09 | 9.875972e-10 | 98.75972 |
| ## A8 | 1.00e-09 | 1.010387e-09 | 101.03865 |
| ## A9 | 1.00e-10 | 9.950654e-11 | 99.50654 |
| ## B6 | 5.00e-09 | 4.954456e-09 | 99.08912 |
| ## B7 | 5.00e-10 | 4.986965e-10 | 99.73930 |
| ## B8 | 1.00e-10 | 9.908095e-11 | 99.08095 |
| ## B9 | 1.00e-10 | 9.934675e-11 | 99.34675 |
| ## Th1 | 7.50e-01 | 7.500000e-01 | 100.00000 |
| ## Th3 | 6.00e+00 | 6.000000e+00 | 100.00000 |
| ## Th4 | 4.50e+00 | 4.500000e+00 | 100.00000 |
| ## E_th1 | 1.00e-01 | 1.000000e-01 | 100.00000 |
| ## E_th3 | 1.00e-01 | 1.000000e-01 | 100.00000 |
| ## E_th4 | 1.30e-01 | 1.300000e-01 | 100.00000 |

TL Fitting



Data fitting for OSL data

```
sequence <- list(OSL = c(125,20,200))
```

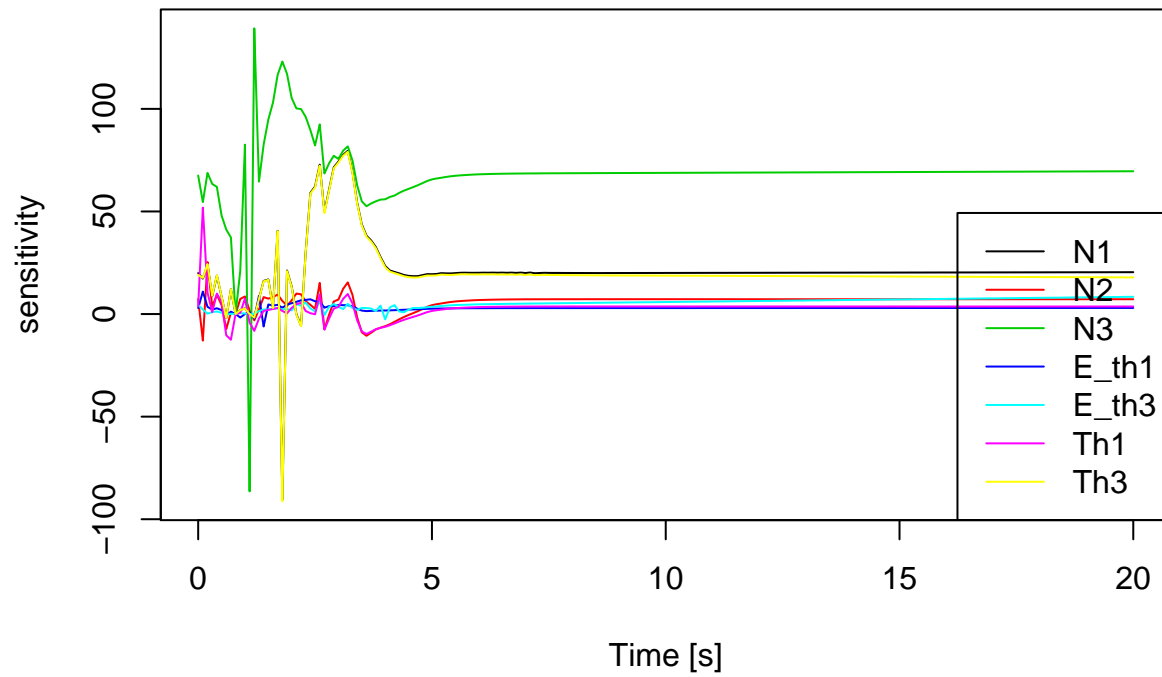
```
model <- "Pagonis2007"
```

```
func_FME <- fit_data2RLumModel(  
  sequence = sequence,  
  model = model,  
  seq.step2fit = 1)
```

```
parms <- extract_pars2FME(model = model)
```

```
SensR <- FME::sensFun(func = func_FME,  
  parms = parms,  
  sensvar = c("signal"),  
  senspar = c("N1", "N2", "N3", "E_th1", "E_th3", "Th1", "Th3")  
)
```

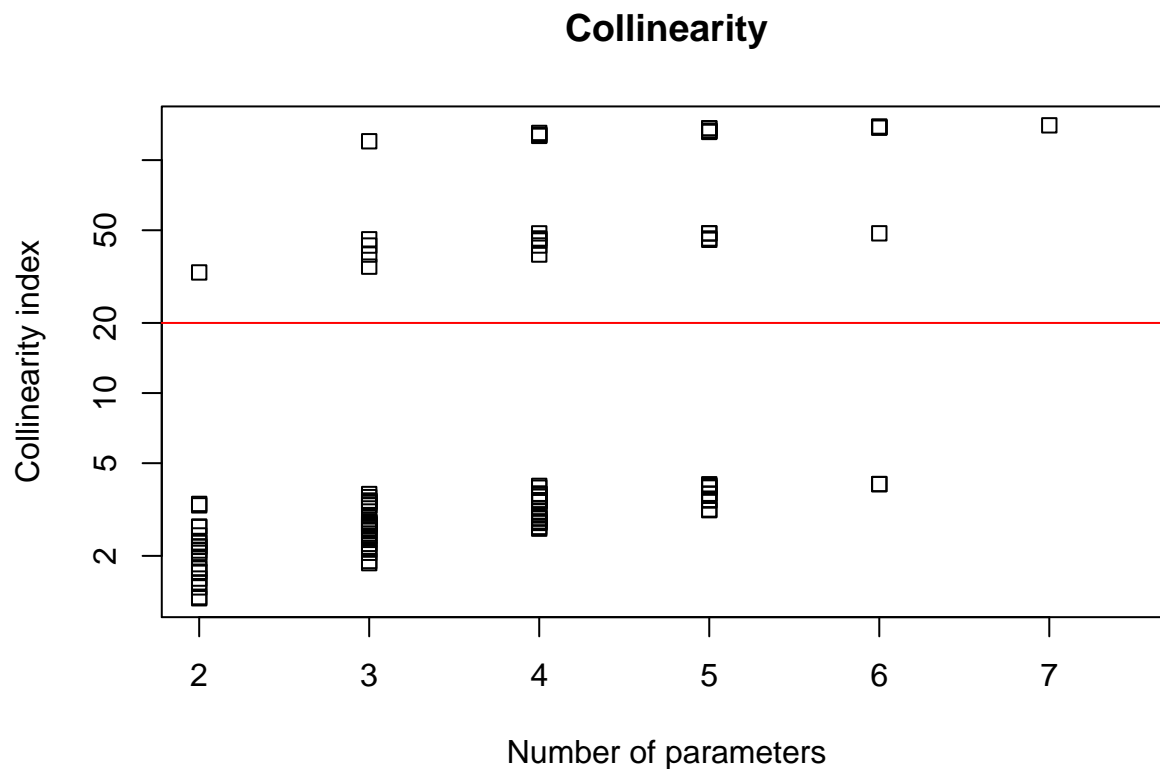
Local Sensitivity Analysis



```
Coll <- FME::collin(SensR)

plot(Coll, log = "y")

abline(h = 20, col = "red") ## 20 = magical number above which there are identifiability problems
```



```
data(ExampleData.CW_OSL_Curve, envir = environment())
exp_data <- CW_Curve.BosWallinga2012
```

```
exp_data[,2] <- exp_data[,2]/max(exp_data[,2])
colnames(exp_data) <- c("time", "signal")
```

```
Fit_func_OSL <- function(x, parset = names(x)){
  parms[parset] <- exp(x)
  out <- func_FME(parms)
  return(modCost(model = out, obs = exp_data))
}
```

```
Fit_OSL <- modFit(f = Fit_func,
  p = log(c(parms[parms != 0])),
  method = "Port")
```

| | old | new | percent |
|-------|---------|--------------|-----------|
| ## N1 | 5.1e+09 | 4977335595 | 97.59482 |
| ## N2 | 1.0e+07 | 9352918 | 93.52918 |
| ## N3 | 1.0e+11 | 98389267042 | 98.38927 |
| ## N4 | 2.5e+08 | 280326320 | 112.13053 |
| ## N5 | 5.0e+10 | 118281876386 | 236.56375 |
| ## N6 | 3.0e+08 | 219576636 | 73.19221 |

OSL Fitting

