

Parameter fitting tool for the TLVP model – User guide

Guide written by:

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Important note




This program is distributed as an executable. Windows Defender (and other antivirus tools) may flag it as a dangerous application as the file has an “Unknown Publisher”.

I assure you it is not dangerous. This program will fit the TLVP parameters to measurement data and write some logs during the process. And nothing else.

This is simply a research tool, and I hope you find it useful in your work.

Installation

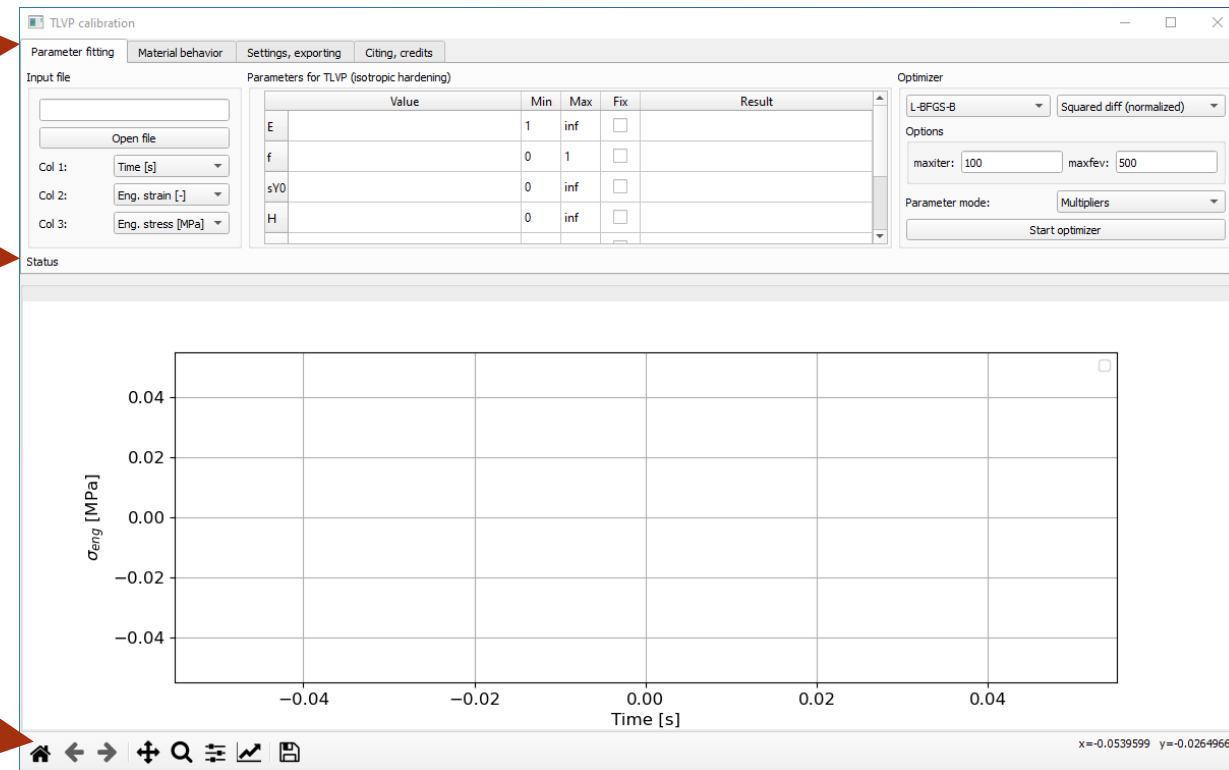
1. Download the executable from the website
 - This is the program itself, no real installation needed
2. Move it into some folder
3. Create folders named „logs” and „exported” in the same folder
 - This is not necessary if the program has permission to create the folders
4. You are done!

| Name | Date modified | Type |
|---|------------------|-------------|
|  exported | 2021-04-22 09:59 | File folder |
|  logs | 2021-04-23 12:08 | File folder |
|  tlv_p_calibration.exe | 2021-04-22 00:14 | Application |

Recommended file structure

Using the program

- Features are organized in groups
- Status messages
- A command window opens with the GUI, don't close it
- Plot controls



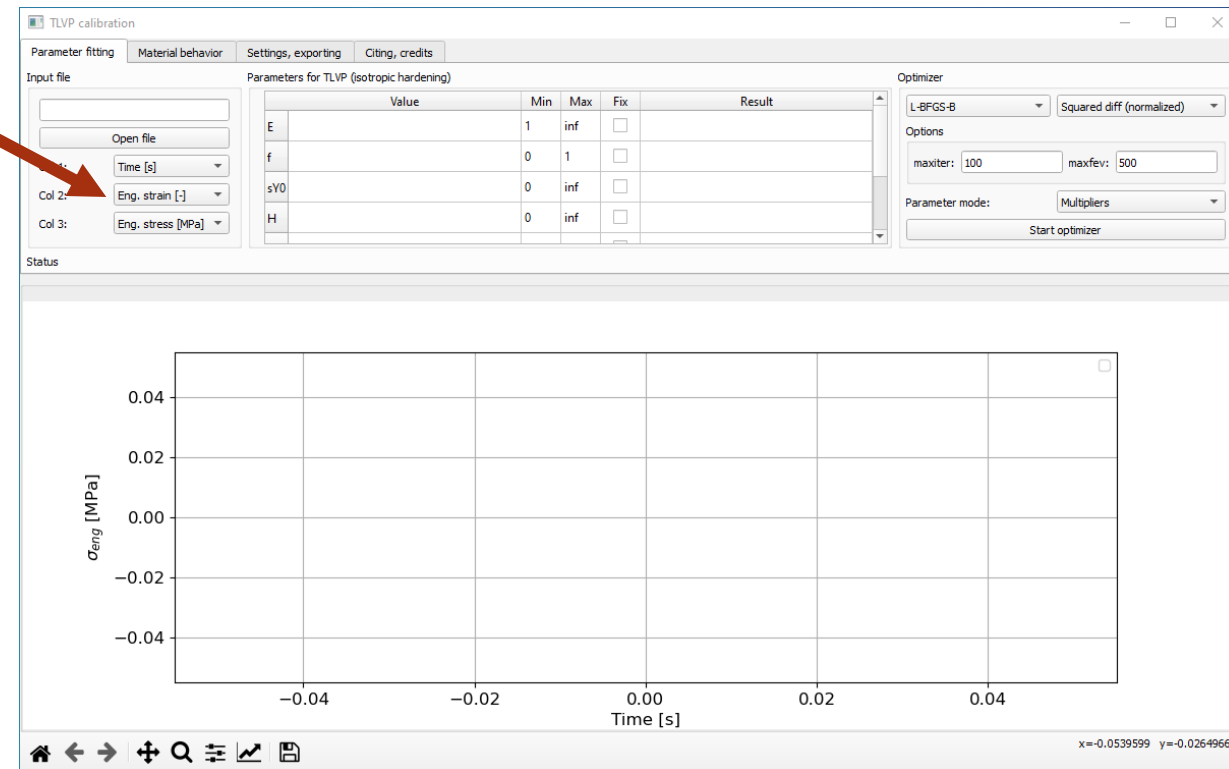
Parameter fitting (1): input file requirements

- .csv (or other text-based) format
- Separator: comma (,)
- Has 3 columns with time, strain, and stress data (additional columns are neglected)
- Time data in increasing order (equality not allowed)
- Lines with the same data as the line before are ignored
- Lines starting with # are ignored
 - You can use this to create headers

```
1 #header
2 #more header
3 0.,0.,0.
4 0.060603565066428104,0.0011993375389573004,0.4344397641987027
5 0.12120712912275561,0.002418403718207551,0.8707333925802879
6 0.18181069418918372,0.00363500383593981,1.2996113391077362
7 0.23236504097846616,0.004631300675787249,1.6475339383800032
8 0.2929686060448943,0.005855299031945852,2.0621983506565416
9 0.35357217010122177,0.0070636788593202195,2.4663571071824077
10 0.4141757351676499,0.008273702750153402,2.851976471207087
11 0.4747792992239774,0.009496057056321283,3.2202924022306596
12 0.5353729996488042,0.010690751416688415,3.5722578198860937
13 0.5959765647152324,0.01191803788629656,3.9121466824078466
14 0.6565801297816605,0.013120663525235303,4.2316422131782945
15 0.7171836938379881,0.014334797554513388,4.539087138822971
16 0.7777872589044161,0.015555507797222453,4.828610651716501
17 0.8383908229607436,0.01674991317273949,5.097122853108685
18 0.8989943880271708,0.017978843692338358,5.353584449375099
19 0.9595979520834984,0.019179003256291016,5.5882622598481255
20 1.0202015171499264,0.020398891474004723,5.811198454279386
21 1.0808050822163544,0.02161466955327353,6.015904246875494
22 1.141408646272682,0.022811541003776654,6.2046970605125775
23 1.20201221133911,0.024039649498380153,6.383602198149027
24 1.2525665581283925,0.025043344590122033,6.5180127937826295
25 1.3131701231948216,0.026252546442491757,6.671580761667458
26 1.3737736872511481,0.027476544798650363,6.813561608843537
27 1.4343772523175753,0.028669306124176674,6.9441098314349
28 1.4949808163739038,0.029898236630307454,7.062452953567473
29 1.555584381440331,0.031100040257718932,7.176624711991773
30 1.61618794650676,0.03231499631199237,7.2870885927068505
31 1.6767915105630866,0.03353488452970607,7.378781337525708
```

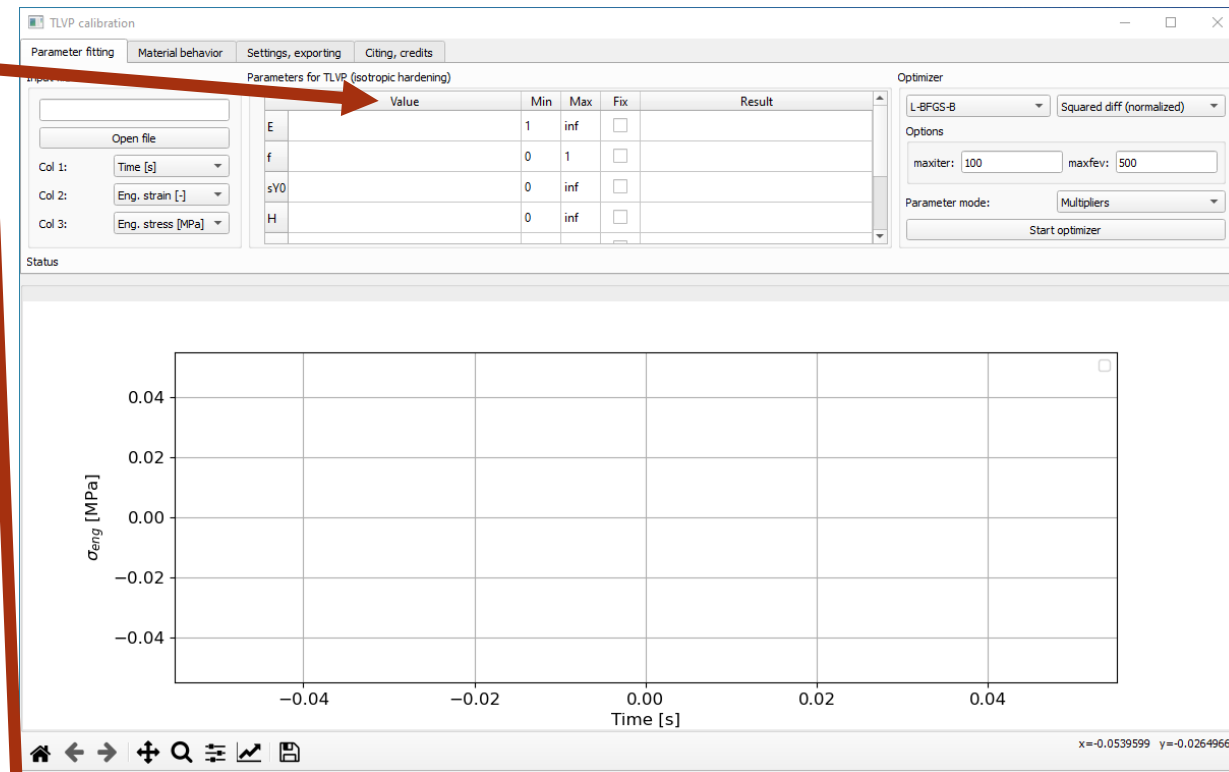
Parameter fitting (2): reading an input file

- The order of the columns in the input has to be given *before* opening the file
- True strain and stress are converted to engineering strain and stress internally
 - Assumption: incompressible material
- Successful input status message:
 - „File read done, valid input“



Parameter fitting (3): initial values

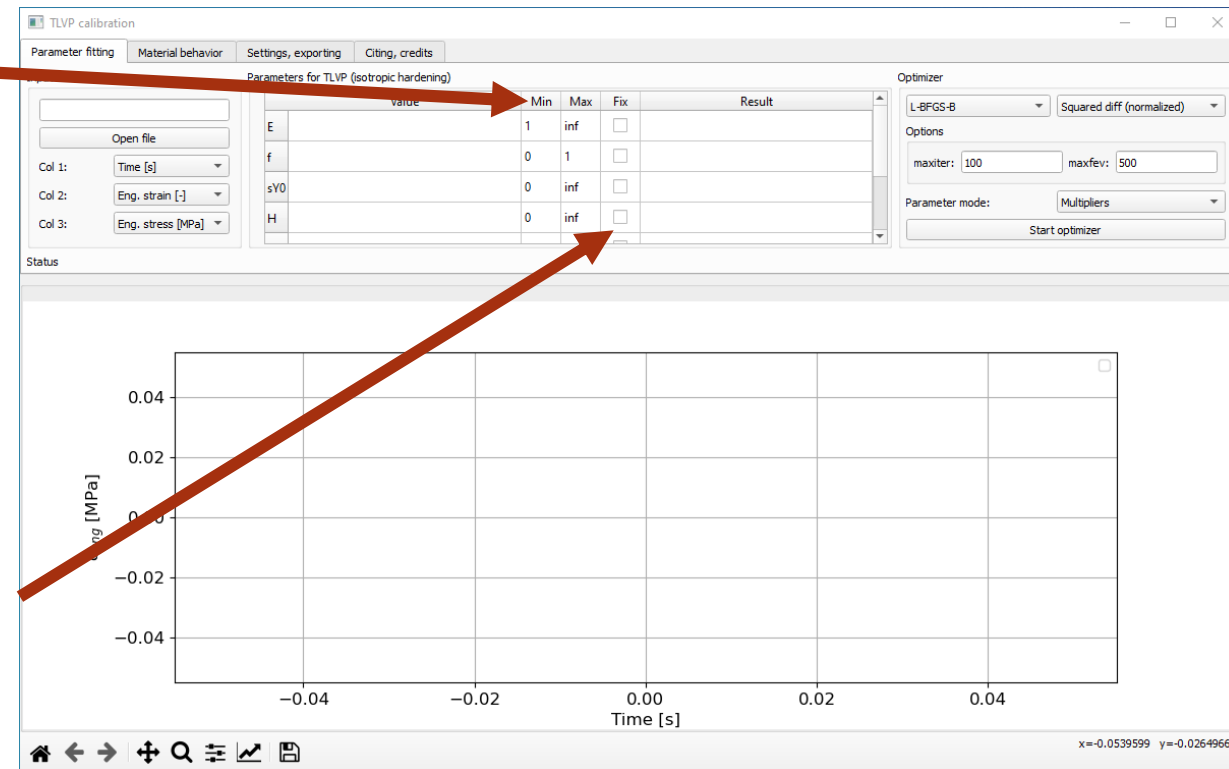
- Initial guess is put in the first column
 - Missing value: filled up from table below
- sY0: better to use a „too low” value, than a „too high” one
 - If sY0 is too high, plastic deformation never starts, the optimizer cannot fit sY0 and H.
 - If sY0=0, plastic deformation is always present, this is also undesirable



| E [MPa] | f [-] | sY0 [MPa] | H [MPa] | $A [MPa^{-n} s^{-m-1}]$ | n [-] | m [-] |
|---------|-------|-----------|---------|-------------------------|-------|-------|
| 1000 | 0.5 | 10 | 100 | 0.001 | 2 | -0.5 |

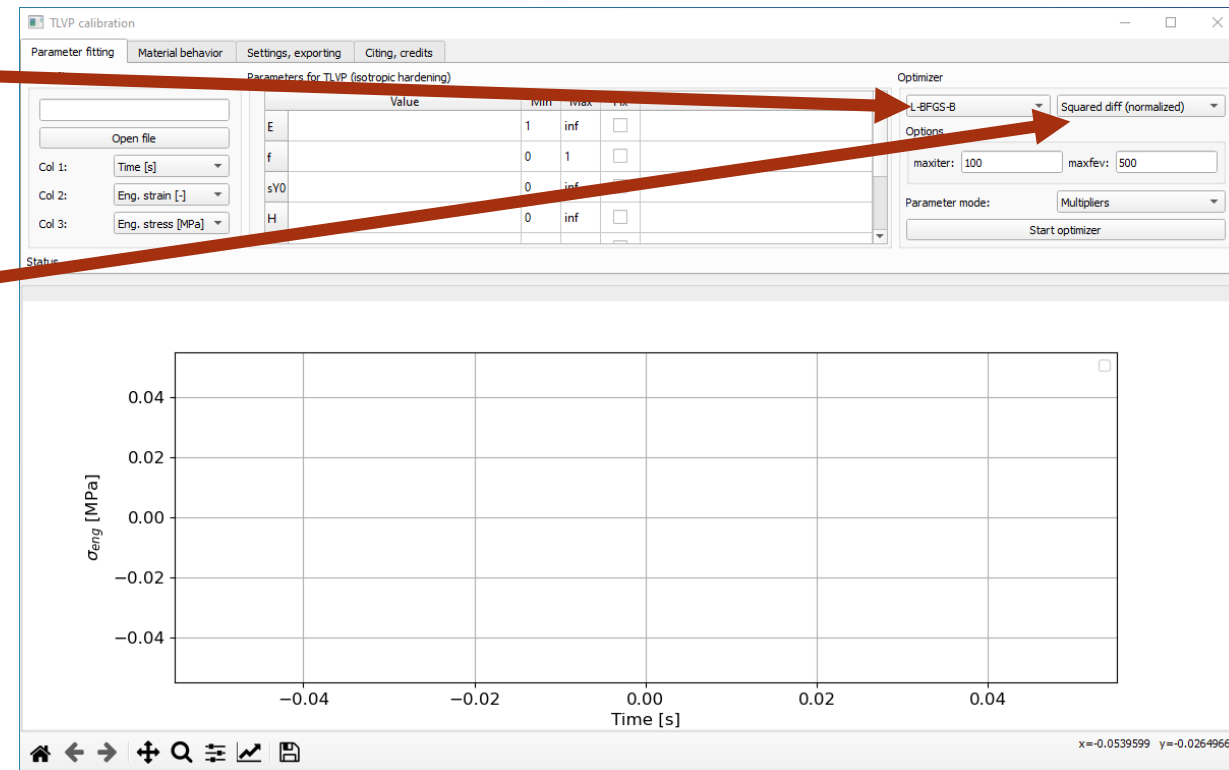
Parameter fitting (4): boundaries, fixing

- Min and max for the optimizers
 - Not all algorithms keep them strictly
- „Focuses the search” in a narrower range
- Too small range:
 - Can lead to stability issues
 - The optimum might not be found, even if it's in the range
- Fix parameter: the optimizer won't change it
 - At least one value must remain changeable
- Note: Ctrl+C and Ctrl+V works in the entire table



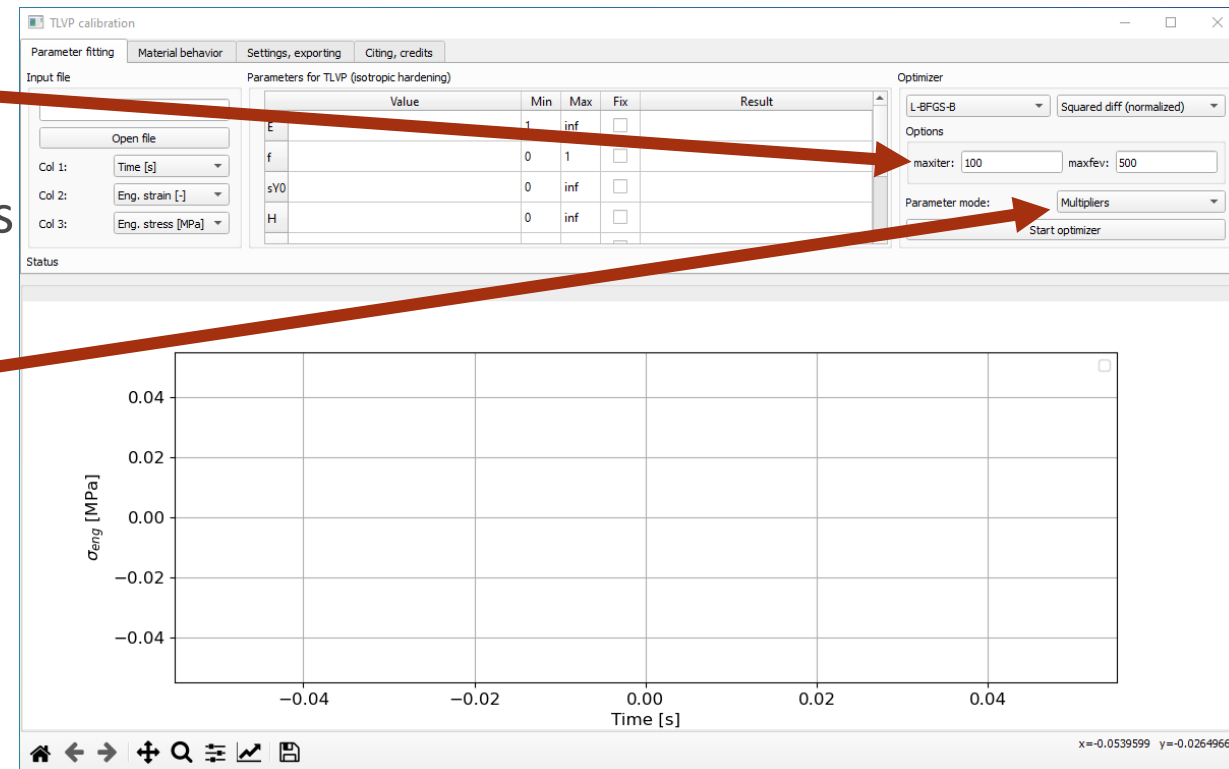
Parameter fitting (5): optimizer settings

- Optimization algorithm
 - Our tests: L-BFGS-B and SLSQP are the „best”, most efficient
 - Documentation: [SciPy](#)
- Quality function:
 - How the difference is measured
 - Absolute and squared difference
 - dX weighted: less weight to densely packed set of points
 - Normalized: normalized with the number of measurement points



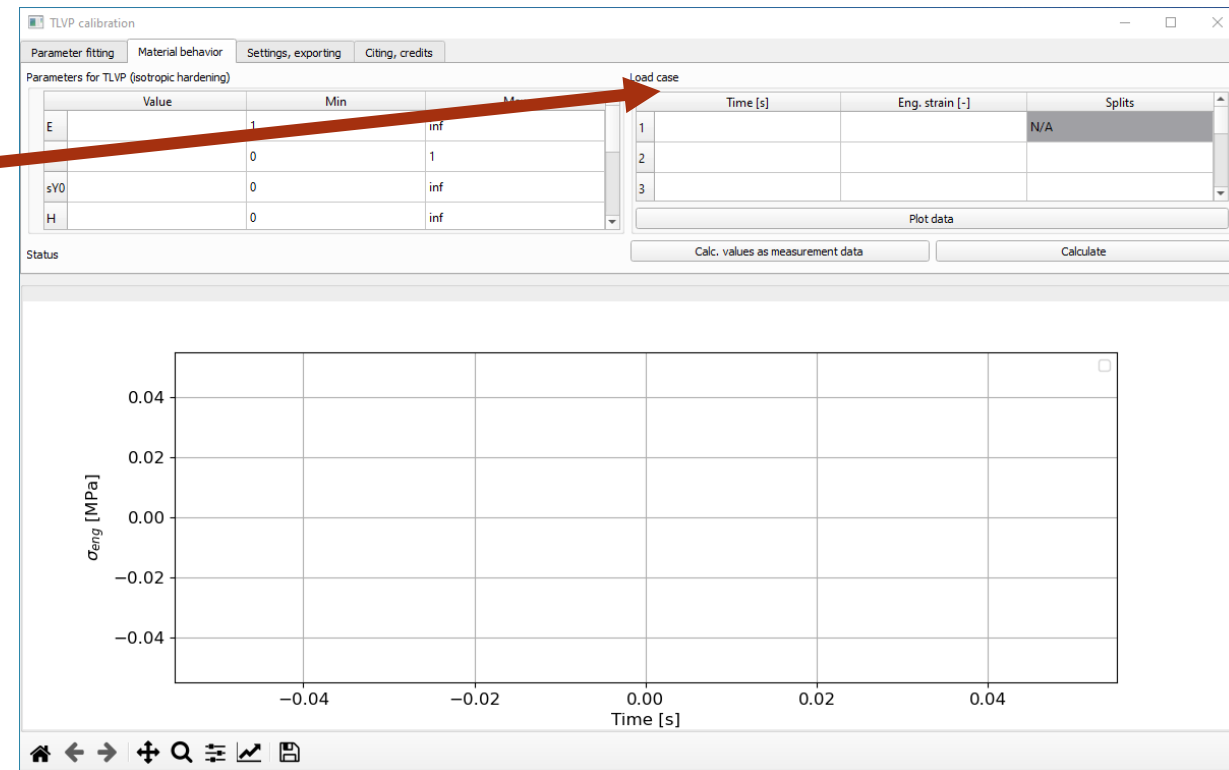
Parameter fitting (6): optimizer settings

- Stopping conditions:
 - Maxiter: max. allowed iterations
 - Maxfev: max. allowed function evaluations (some algorithms ignore it)
 - The optimizer stops if either is met
- Parameter mode:
 - Values: the parameters are optimized directly. Not recommended.
 - Multipliers: initial guesses are used as internal multipliers. The optimizer „sees” values in more similar magnitudes
 - Normalized: parameters are transformed to the [0,1] range based on their boundaries



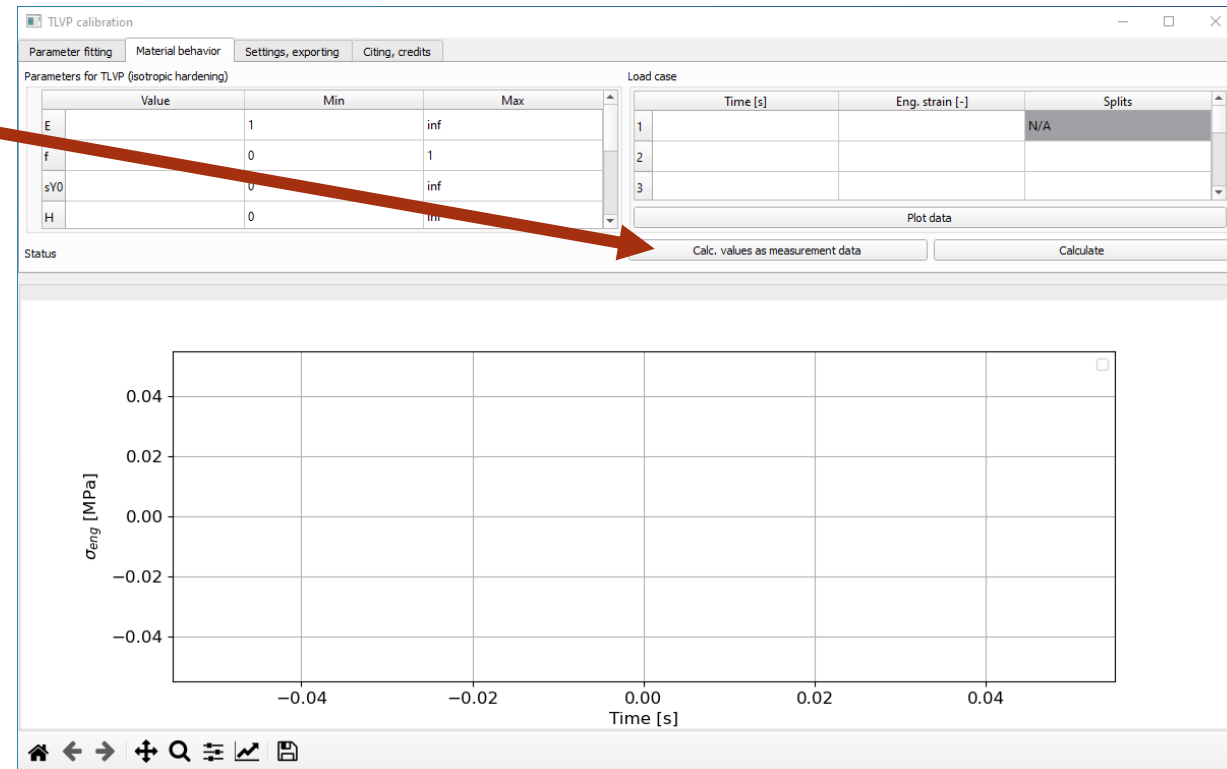
Material behavior (1): general

- Values are give directly
 - Boundaries only serve as reminders
- Uniaxial load:
 - Time-engineering strain history given by points (linear path assumed in between)
 - Number of division between points: 3rd column (must be >0 integer)
 - The „Plot data” only plots the load specified in the table
- If the table has no valid load data:
 - The measured strain history is used (if a measurement file was loaded)



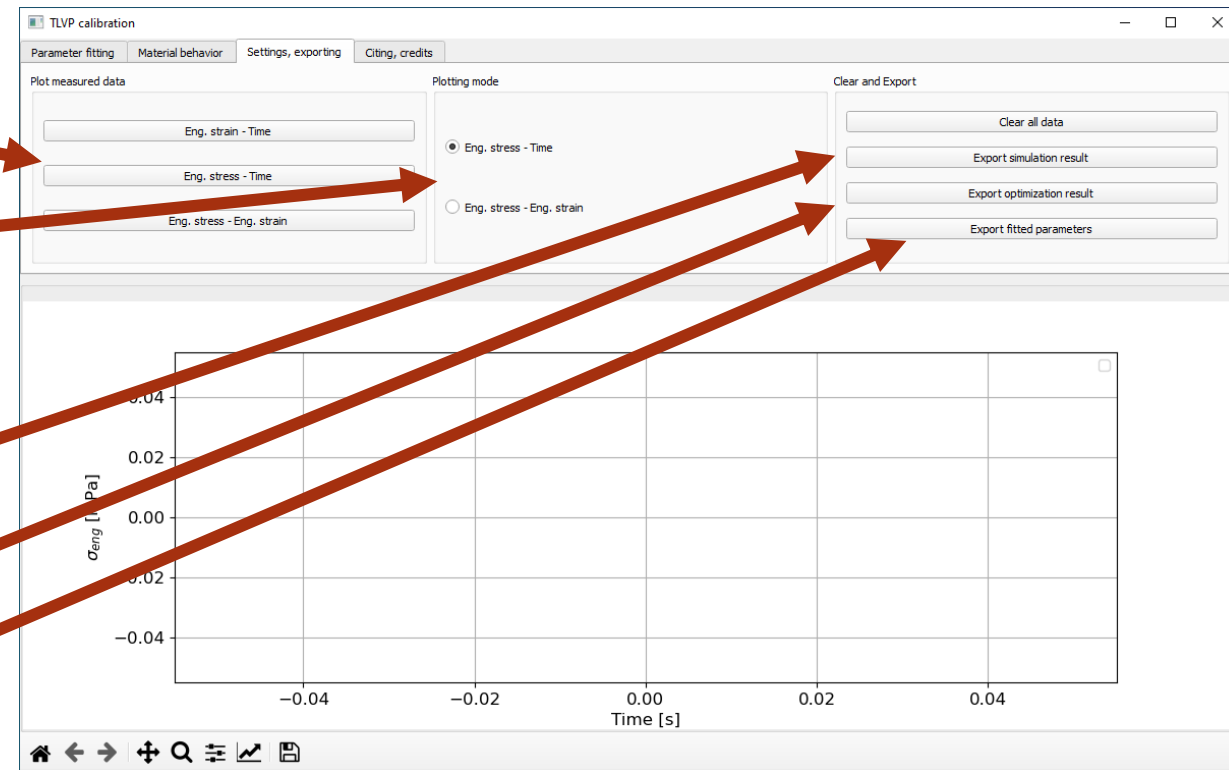
Material behavior (2): testing of optimizers

- Results can be interpreted as measurement data
- Test the optimizer settings in the first tab, while knowing the exact values it should converge to



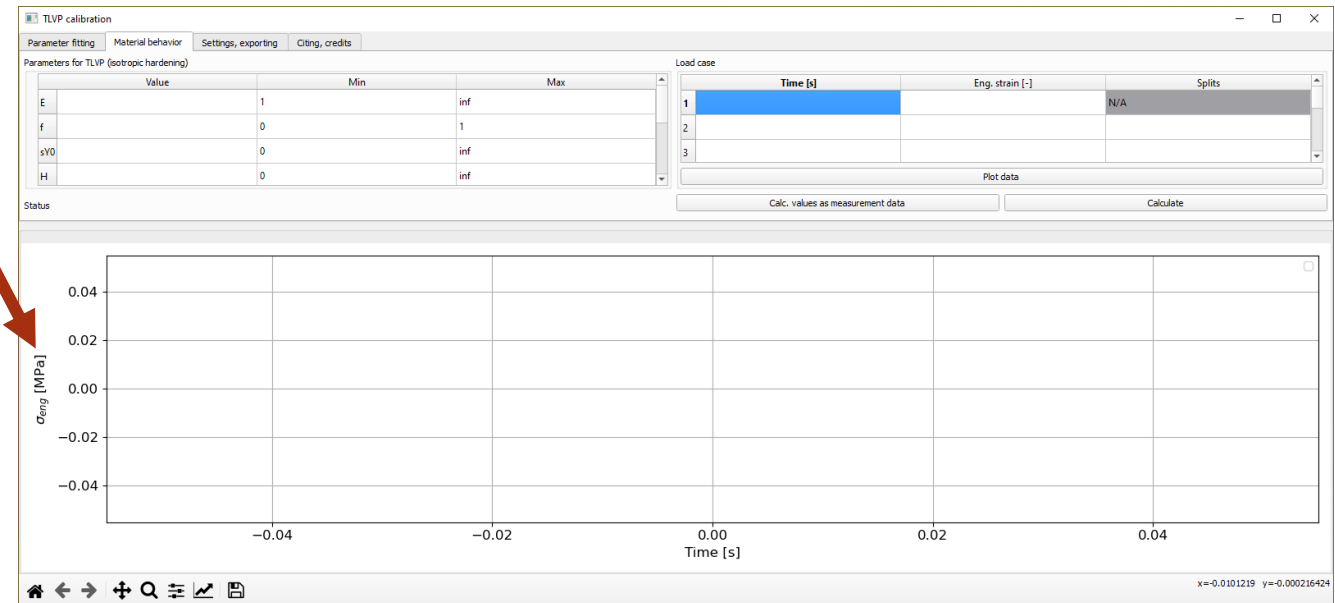
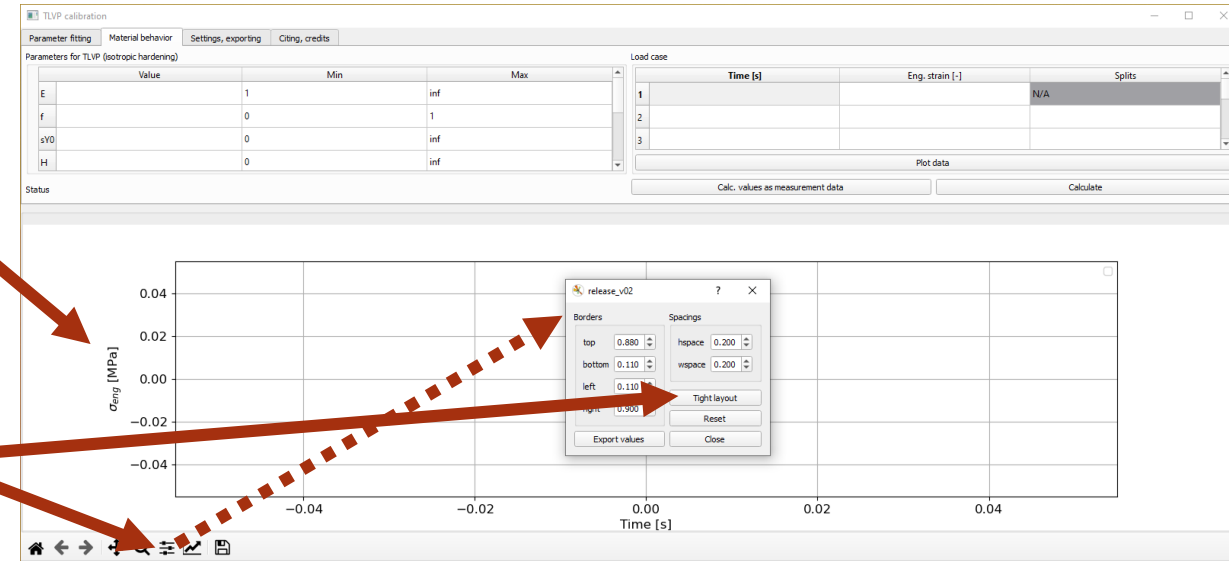
Settings, exporting

- Plot the measured data
- X axis: time or strain data
 - Cannot be changed during optimization
- Clear all data:
 - Forget about the loaded values
- Export results from the material behavior tab
- Export the fitted and measured behavior
- Export fitted parameters
- Files are put in the „exported” folder



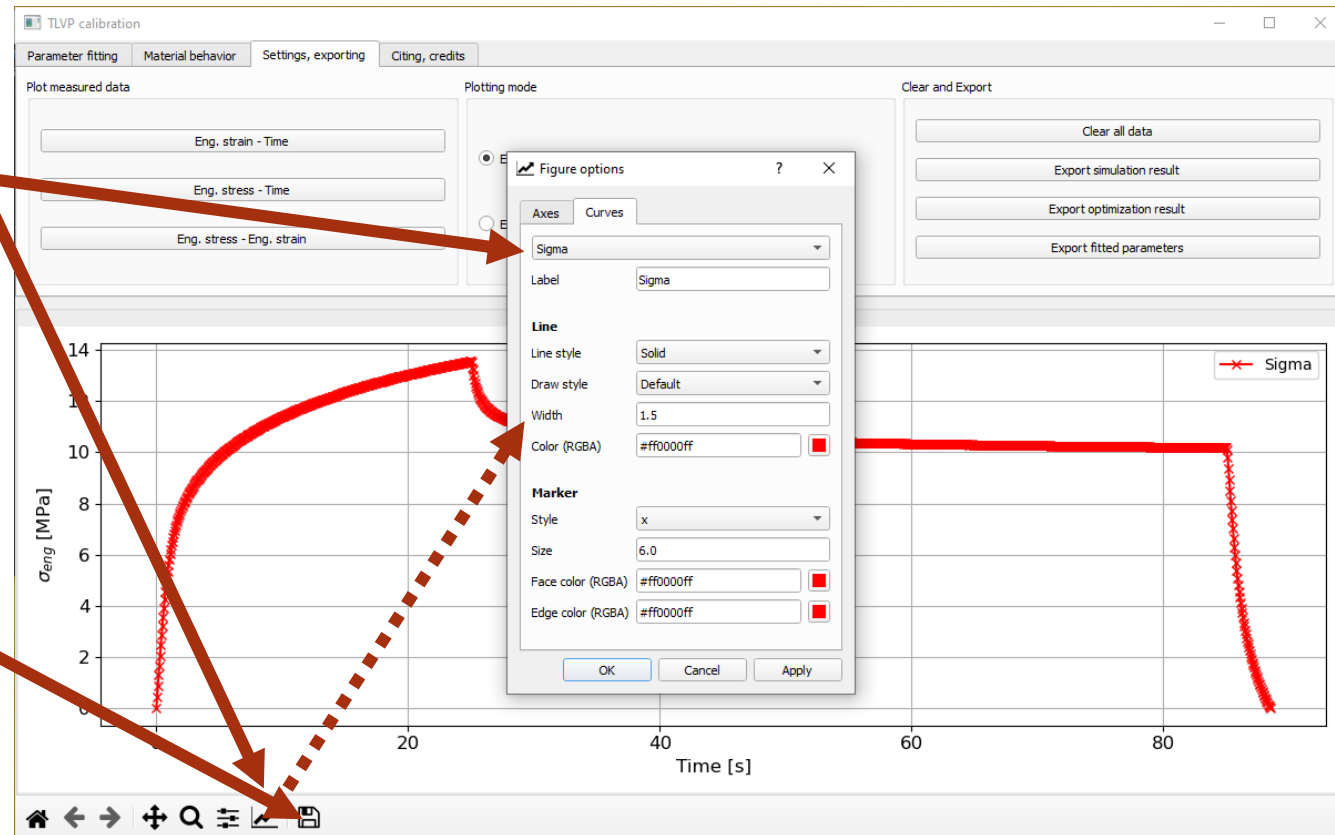
Tips (1): fixing axis labels

- Sometimes labels are placed incorrectly
 - Should be at the edge of the window
- 1. Bottom menu, configure subplots
- 2. „Tight layout” button
- 3. Labels moved to correct positions



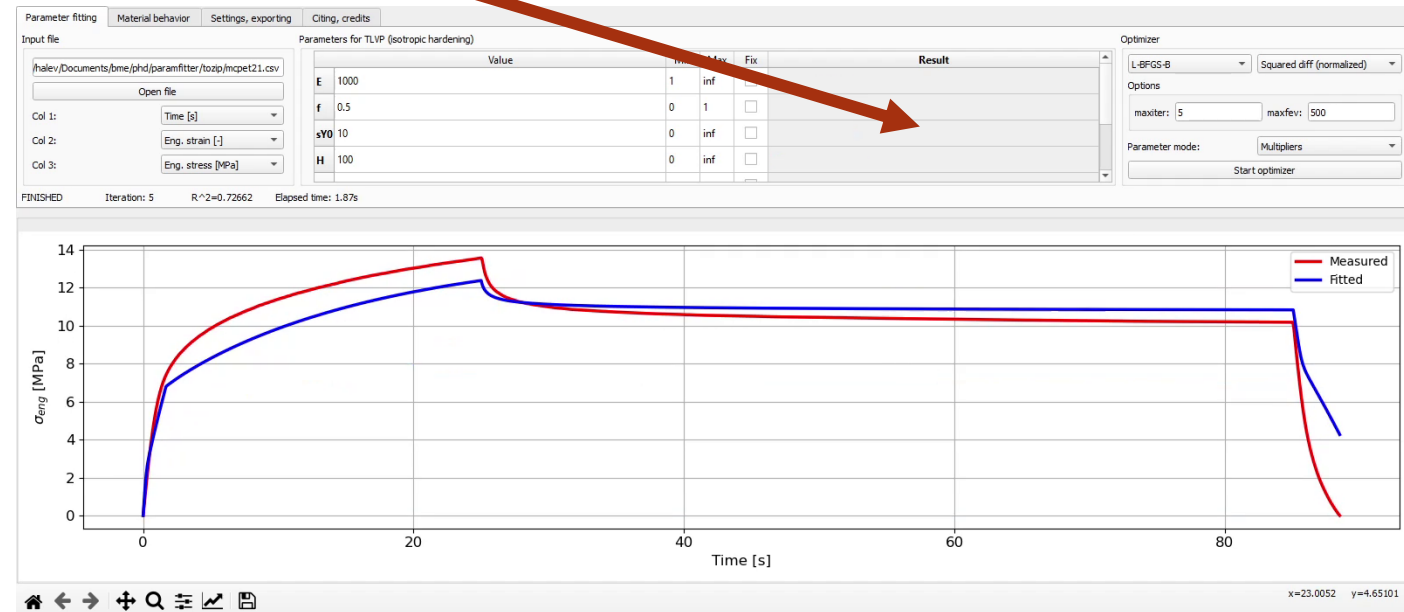
Tips (2): Changing curve properties

1. Bottom menu, edit axes, curve...
 2. Select the curve
 3. Edit properties (line width, markers, etc)
- Note: these settings are reset when replotting
 - Save the figure (several formats)




Tips (3): result column not rendering/updating

- Sometimes the values in the result column don't show up or update
 - Only when using Windows
- Solution:
 - Click into the cells
 - Select the column header
 - Use the scrollbar



Parameter fitting: An example

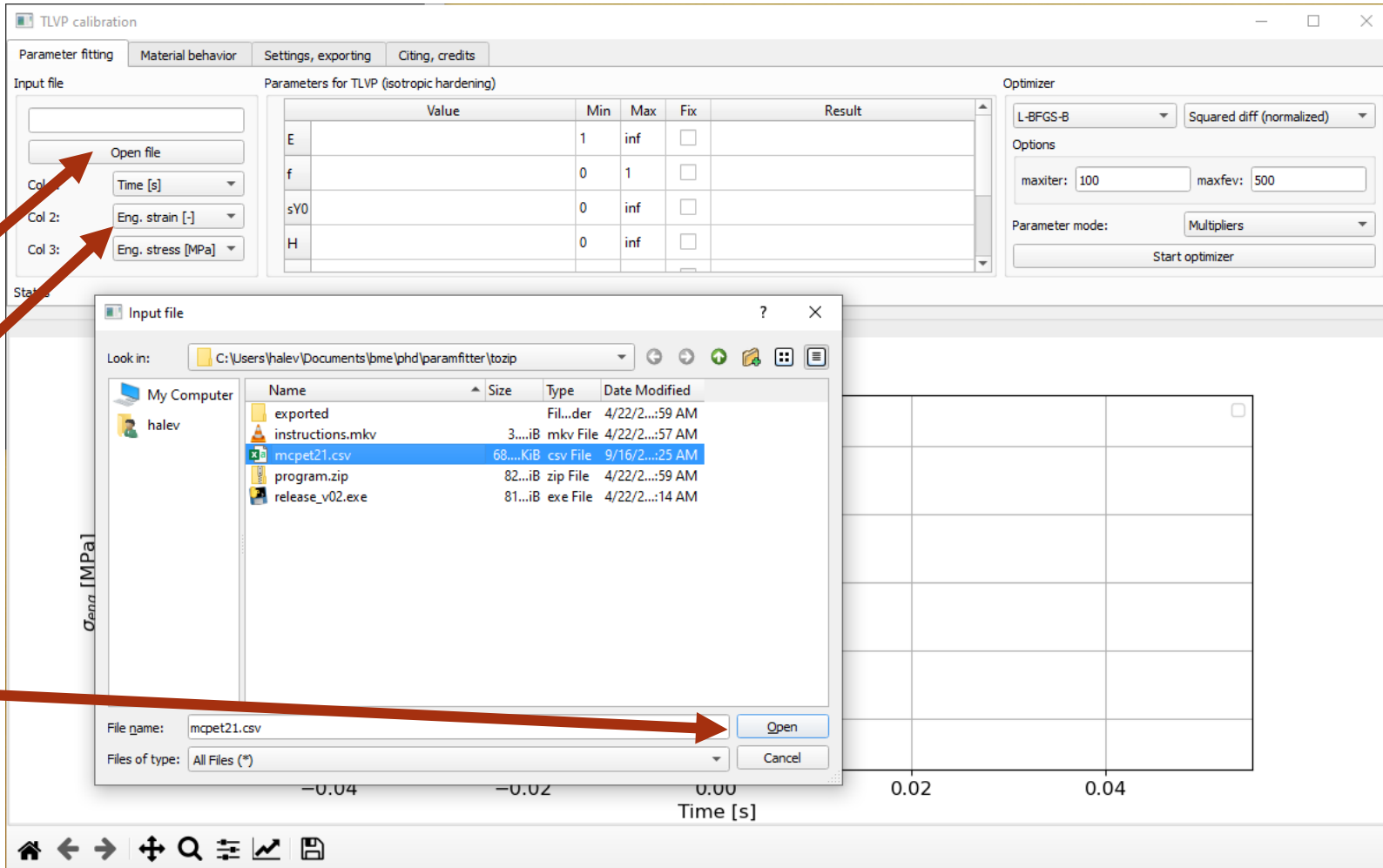


Goal

- Show a fitting example using real measurement data
 - Measured material: MC-PET at room temperature
- Show how to judge the obtained results

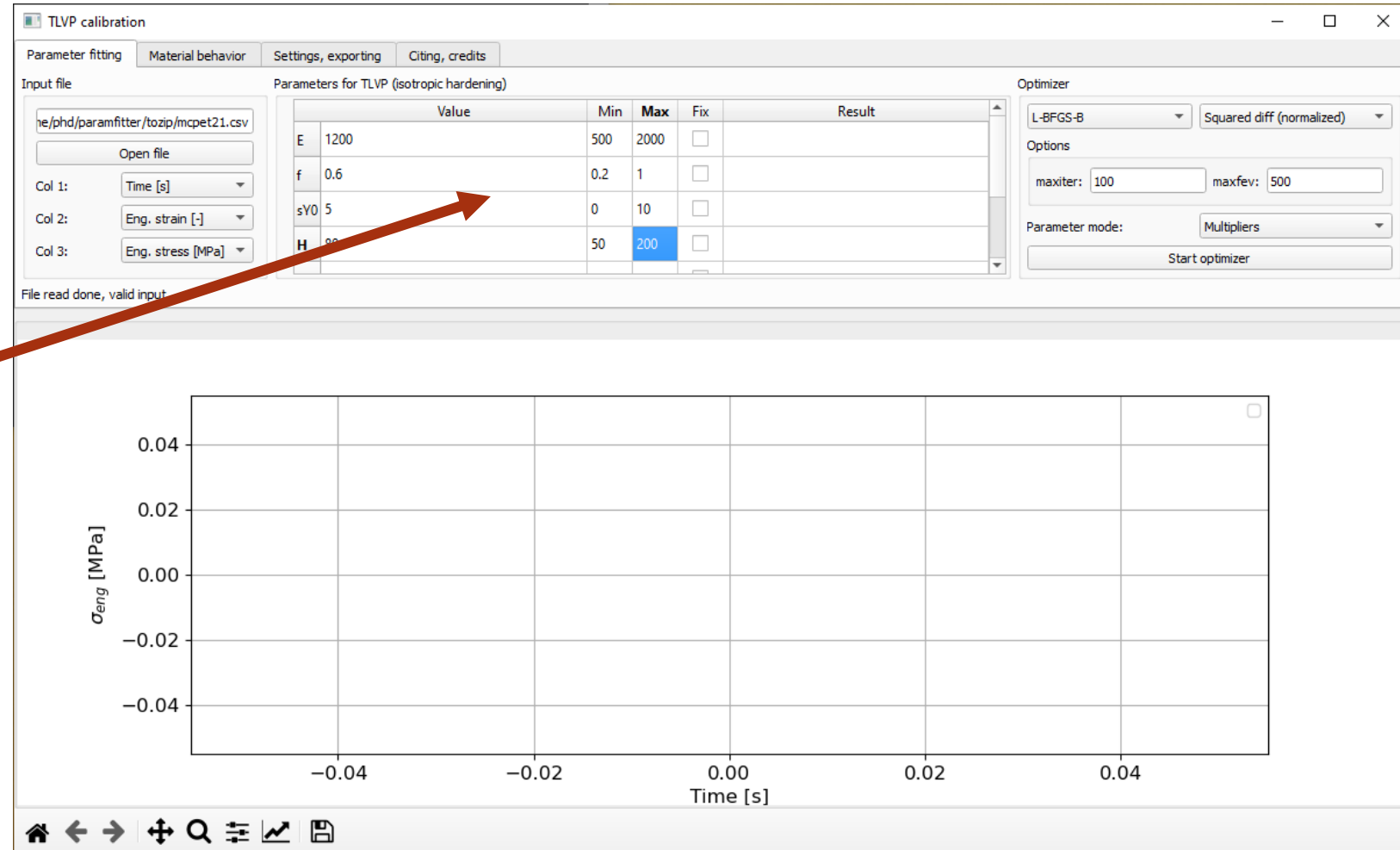
Start the program, load the measurement file

- Measured material: MC-PET @ room temperature
 - Known: column order
1. Setup column order
 2. Open file
 3. Open



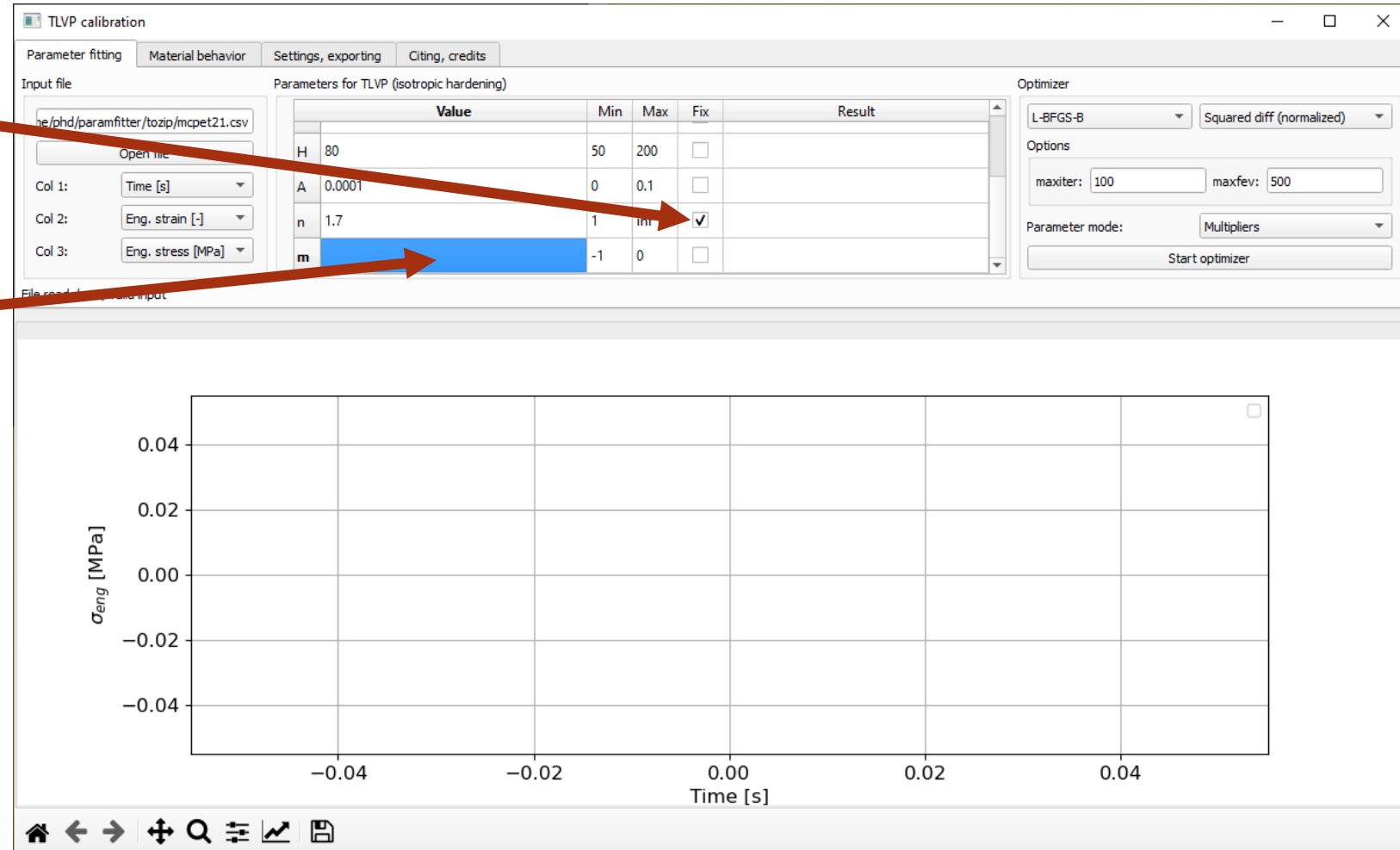
Initial guess (1)

- We have following ideas for some parameters before starting (values; ranges):
 - $E \approx 1200$; $500 < E < 2000$
 - $f \approx 0.6$; $0.2 < f < 1$
 - $sY0 \approx 5$; $0 < sY0 < 10$
 - $H \approx 80$; $50 < H < 200$
 - $A \approx 0.0001$; $0 < A < 0.1$



Initial guess (2)

- For some reason we are certain that $n=1.7$ -> fix
- We have no idea about m -> leave the field empty
 - The program will fill in the default value of $m \approx -0.5$



Optimizer settings

- Let's use the SLSQP algorithm
- Start the optimizer

The screenshot shows the TLVP calibration software interface. The 'Optimizer' tab is active, displaying the following settings:

- Optimizer: SLSQP
- Method: Squared diff (normalized)
- Options: maxiter: 100, maxfev: 500
- Parameter mode: Multipliers
- Start optimizer button

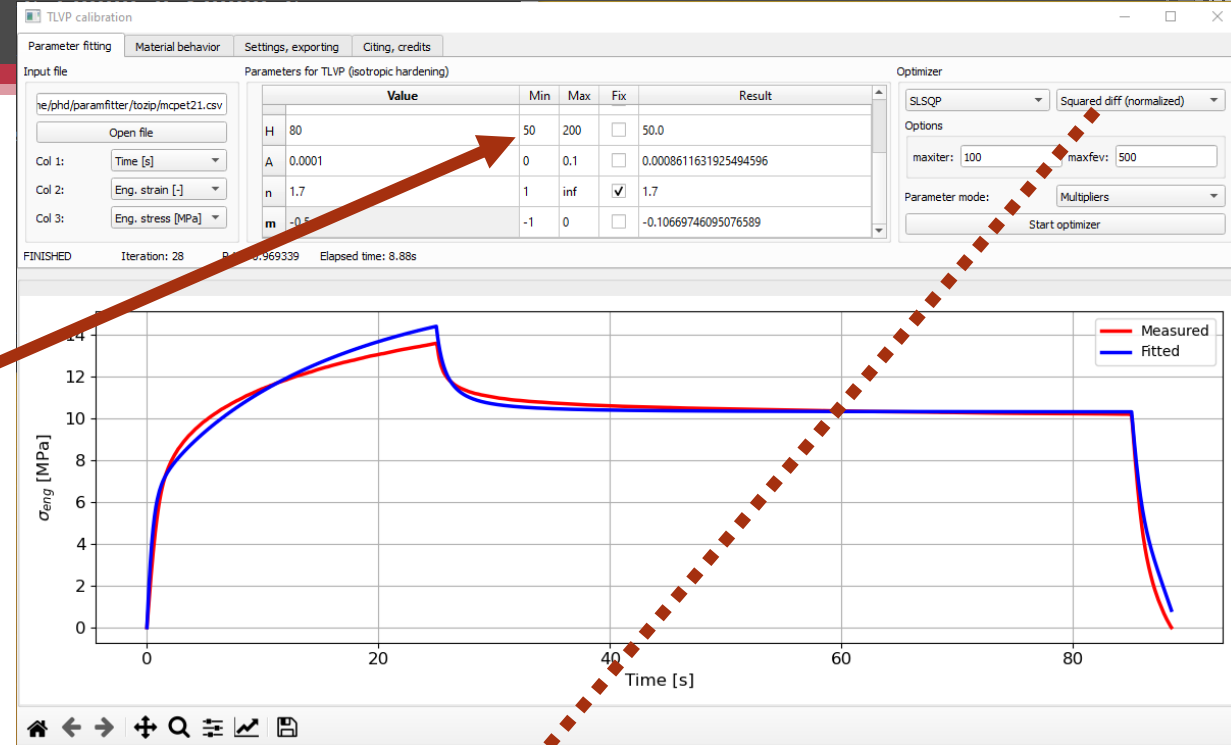
The 'Parameter fitting' tab shows a table of parameters:

| Parameter | Value | Min | Max | Fix |
|-----------|--------|-----|-----|-------------------------------------|
| H | 80 | 50 | 200 | <input type="checkbox"/> |
| A | 0.0001 | 0 | 0.1 | <input type="checkbox"/> |
| n | 1.7 | 1 | inf | <input checked="" type="checkbox"/> |
| m | | -1 | 0 | <input type="checkbox"/> |

The plot area shows a graph of engineering stress σ_{eng} [MPa] versus Time [s]. The y-axis ranges from -0.04 to 0.04, and the x-axis ranges from -0.04 to 0.04. The plot is currently empty.

Check results

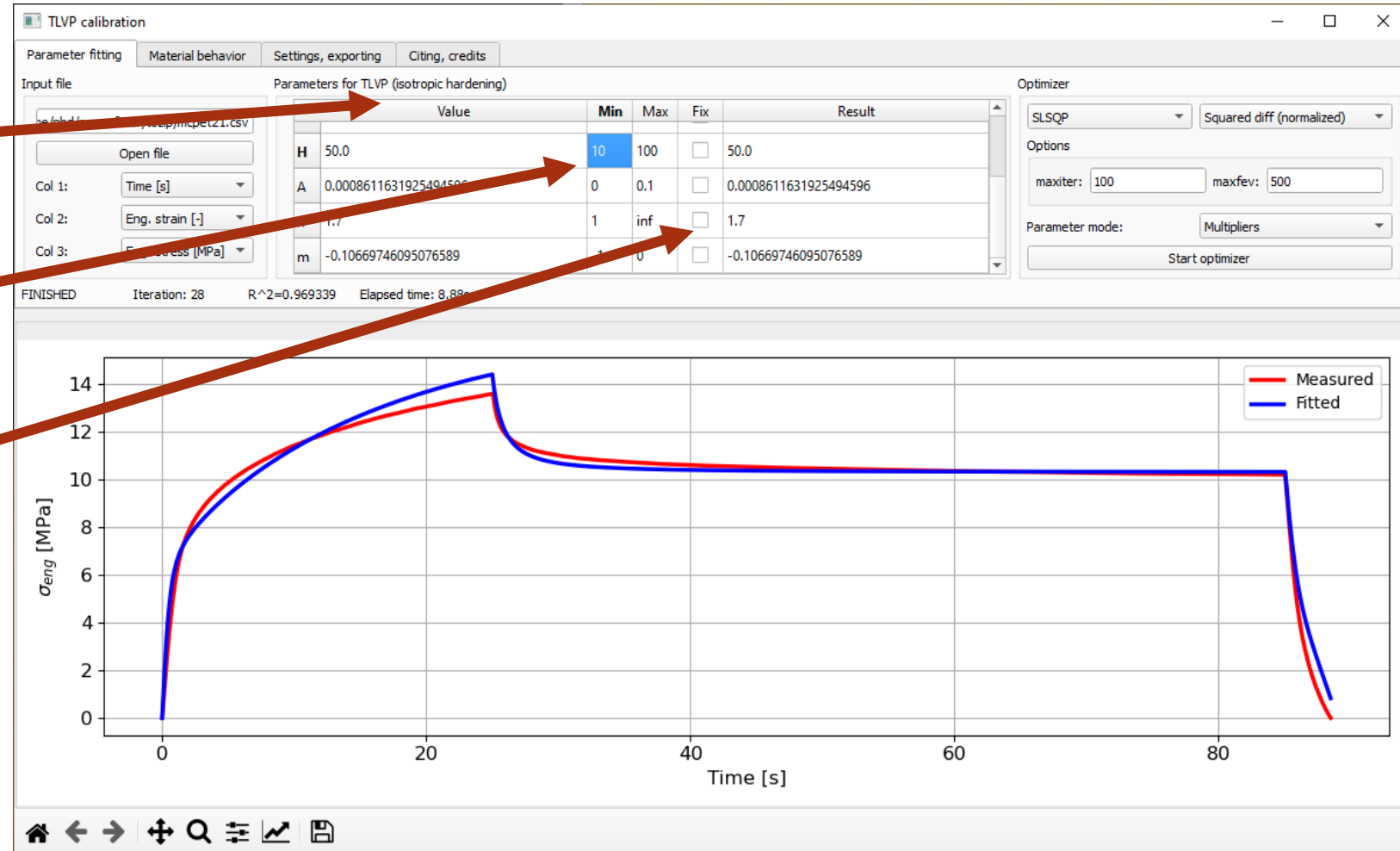
- Did we „hit” any boundaries?
 - Yes, $H=50$ in the results, our initial guessed range was probably wrong
- The console also has useful information:
 - The optimizer „terminated successfully”, it didn't reach the maxiter or maxfev limit
 - The final value of the normalized squared differences was 0.363
- Conclusion: let's try again with different boundaries for H



```
C:\Users\halev\Documents\bme\phd\paramfitter\tozip\release_v2.exe
Current material parameters: [ 7.13861430e+02  7.77426630e-01  0.00000000e+00  5.00000000e+01
 8.65352297e-04  1.70000000e+00 -1.07425107e-01]
Current optimizer parameters: [5.99443161e-01  1.29854101e+00  1.48578304e-16  6.25000000e-01
 8.63853520e+00  2.15018805e-01]
Current material parameters: [ 7.19331800e+02  7.79124604e-01  7.42891521e-16  5.00000000e+01
 8.63853520e-04  1.70000000e+00 -1.07509403e-01]
Current optimizer parameters: [0.59993914  1.29882913  0.        0.625  8.61163193  0.21339492]
Current material parameters: [ 7.19926971e+02  7.79297479e-01  0.00000000e+00  5.00000000e+01
 8.61163193e-04  1.70000000e+00 -1.06697461e-01]
Current optimizer parameters: [0.59993914  1.29882913  0.        0.625  8.61163193  0.21339492]
Current material parameters: [ 7.19926971e+02  7.79297479e-01  0.00000000e+00  5.00000000e+01
 8.61163193e-04  1.70000000e+00 -1.06697461e-01]
None
THREAD COMPLETE!
fun: 0.36309804027373693
jac: array([ 1.26779079e-03, -1.52513012e-03,  2.84065470e-01,  1.60495654e+00,
 9.42051411e-05, -5.06121665e-04])
message: 'Optimization terminated successfully.'
nfev: 245
nit: 29
njev: 28
status: 0
success: True
x: array([0.59993914, 1.29882913, 0.        , 0.625  , 8.61163193,
 0.21339492])
Number of function evaluations: 245
***FINAL PLOT
Current material parameters: [ 7.19926971e+02  7.79297479e-01  0.00000000e+00  5.00000000e+01
 8.61163193e-04  1.70000000e+00 -1.06697461e-01]
```

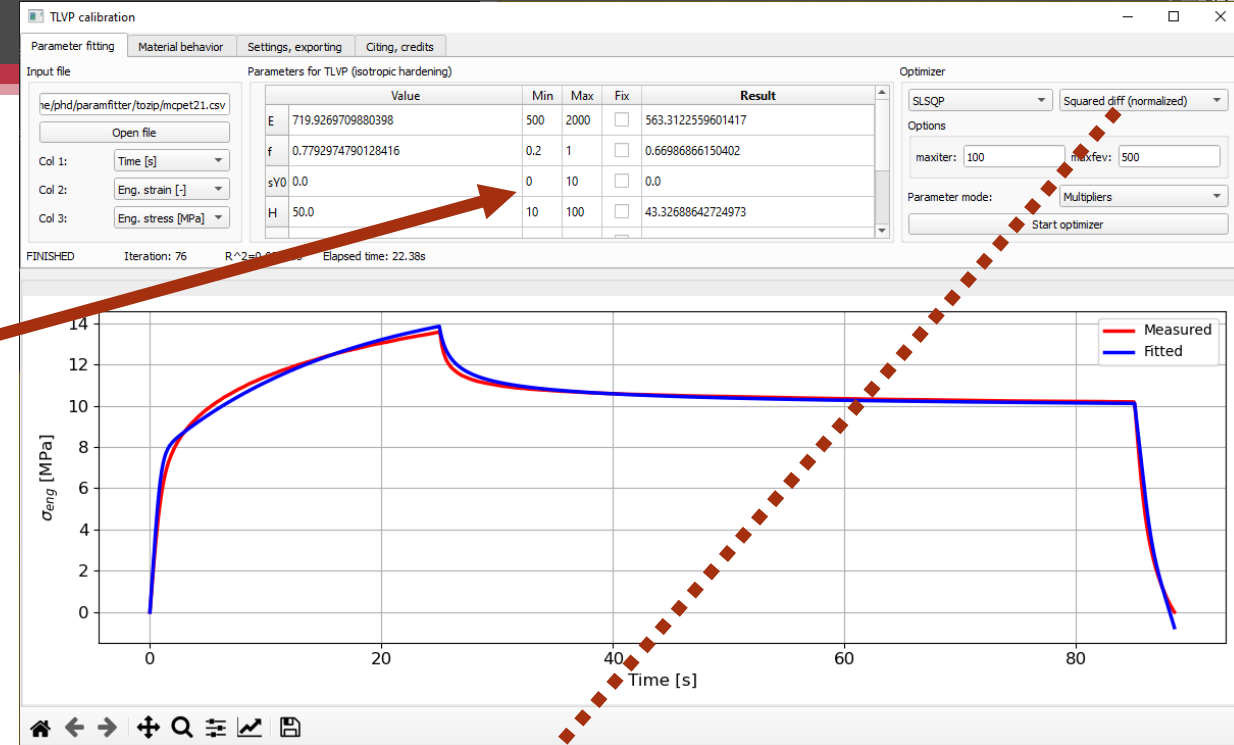
Retry

- Let's use the old results as the initial guess:
 - Ctrl+C, Ctrl+V the values
- Change the limits of H to $10 < H < 100$
- Let's try with removing the „fix” from n
- Restart!



Check results again

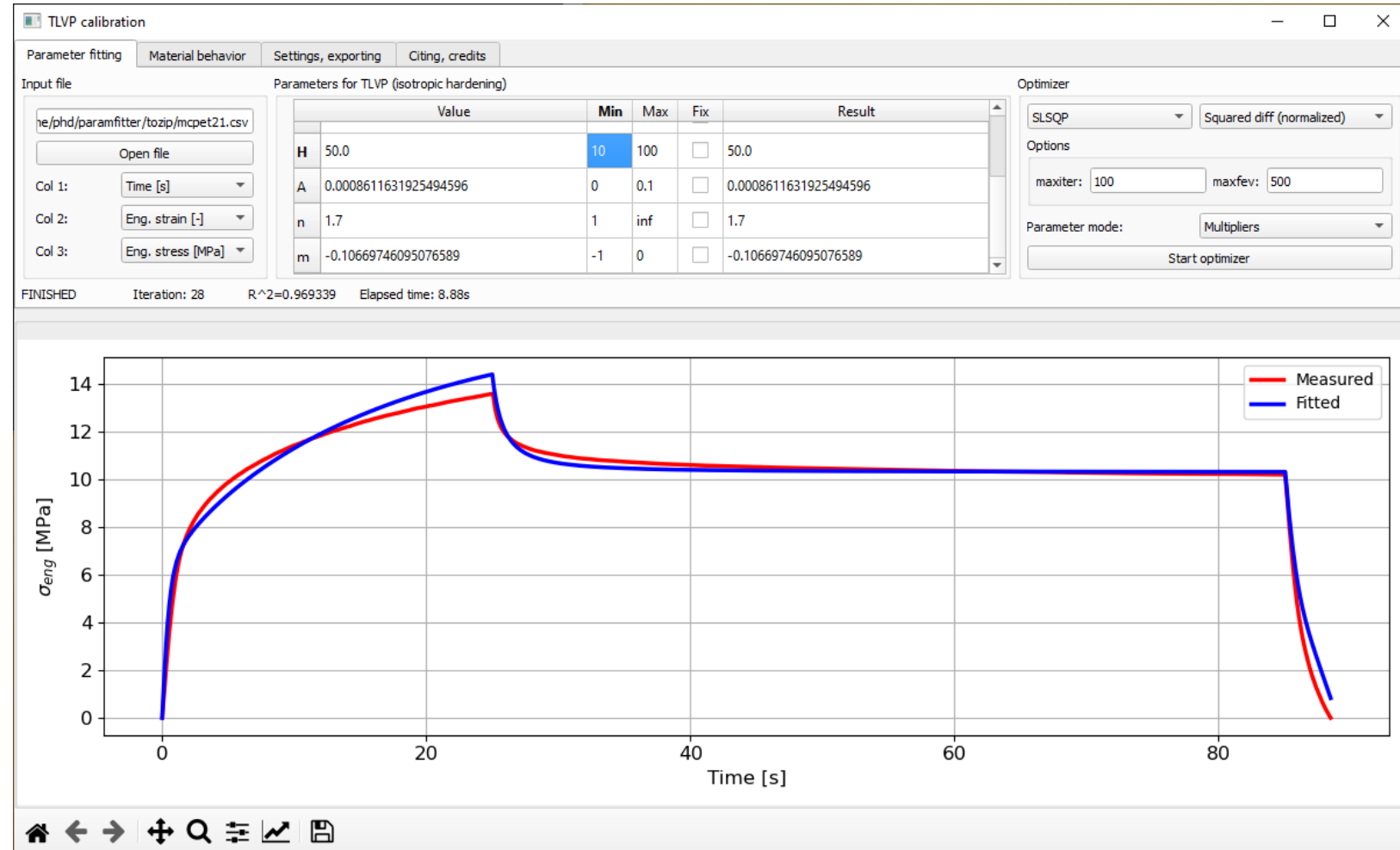
- Did we „hit” any boundaries?
 - Yes, $sY0=0$ in the results
- The console also has useful information:
 - The optimizer „terminated successfully”, it didn’t reach the maxiter or maxfev limit (well, actually SLSQP ignores maxfev...)
 - The final value of the normalized squared differences was 0.21
- Conclusion: let’s try again with changing $sY0$ ’s initial guess



```
C:\Users\halev\Documents\bme\phd\paramfitter\tozip\release_v02.exe
Current optimizer parameters: [0.78295516 0.85911659 1. 0.86679852 0.02650965 2.00106339
0.]
Current material parameters: [ 5.63670534e+02 6.69507395e-01 0.00000000e+00 4.33399261e+01
2.28291325e-05 3.40180776e+00 -0.00000000e+00]
Current optimizer parameters: [0.7824575 0.85958017 1. 0.86653773 0.02589014 2.00758704
0.]
Current material parameters: [ 5.63312256e+02 6.69868662e-01 0.00000000e+00 4.33268864e+01
2.22956357e-05 3.41289797e+00 -0.00000000e+00]
Current optimizer parameters: [0.7824575 0.85958017 1. 0.86653773 0.02589014 2.00758704
0.]
Current material parameters: [ 5.63312256e+02 6.69868662e-01 0.00000000e+00 4.33268864e+01
2.22956357e-05 3.41289797e+00 -0.00000000e+00]
None
THREAD COMPLETE!
fun: 0.21057411354977357
jac: array([ 0.00244917, -0.00497693, 0. , 0.00906569, -0.06944477,
-0.00555753, 0.00402821])
message: 'Optimization terminated successfully.'
nfev: 710
nit: 76
njev: 76
status: 0
success: True
x: array([0.7824575 , 0.85958017, 1. , 0.86653773, 0.02589014,
2.00758704, 0. ])
Number of function evaluations: 710
****FINAL PLOT
Current material parameters: [ 5.63312256e+02 6.69868662e-01 0.00000000e+00 4.33268864e+01
2.22956357e-05 3.41289797e+00 -0.00000000e+00]
```

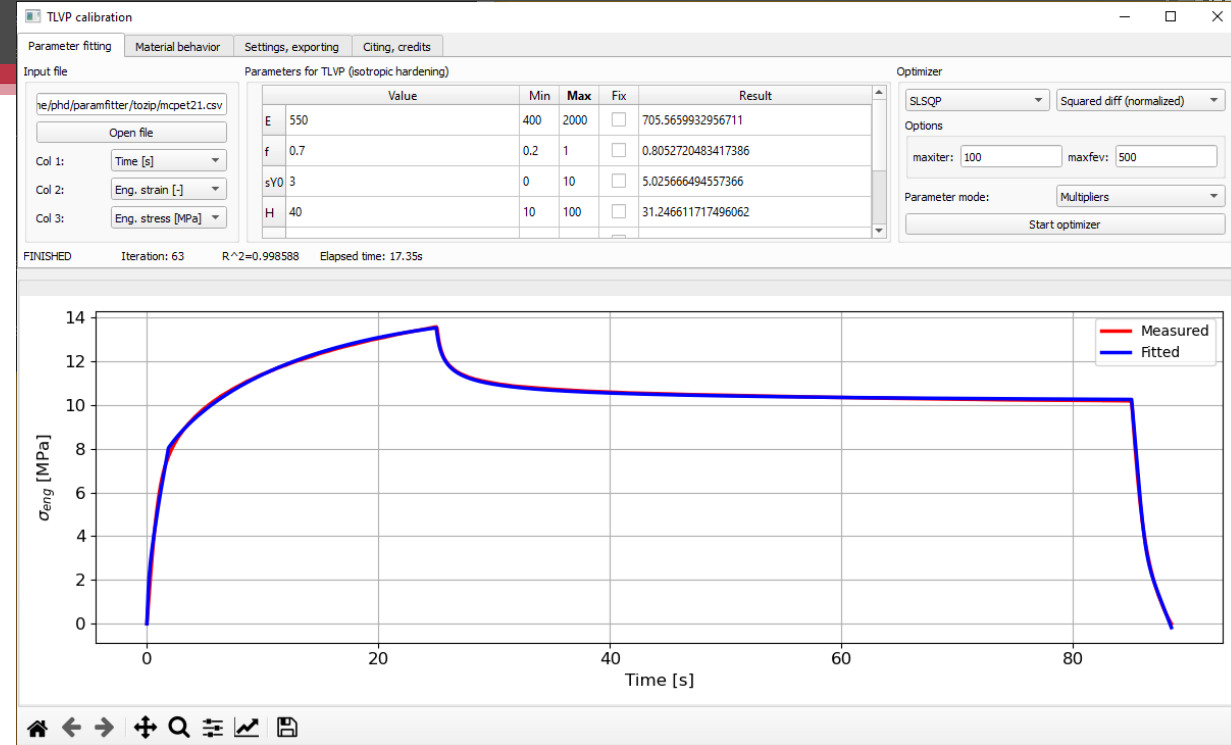
Retry 2

- Let's base the new initial guess on the results
- Perturb the initial guess:
 - Change the copied values slightly (about +/- 10%) to help avoiding local minima
 - $E \approx 550$; $400 < E < 2000$
 - $f \approx 0.7$; $0.2 < f < 1$
 - $sY0 \approx 3$; $0 < sY0 < 10$
 - $H \approx 40$; $10 < H < 200$
 - $A \approx 2e-5$; $0 < A < 0.1$
 - $n \approx 3$; $1 < n < 10$
 - $m \approx -0.5$; $-1 < m < 0$



Check results again

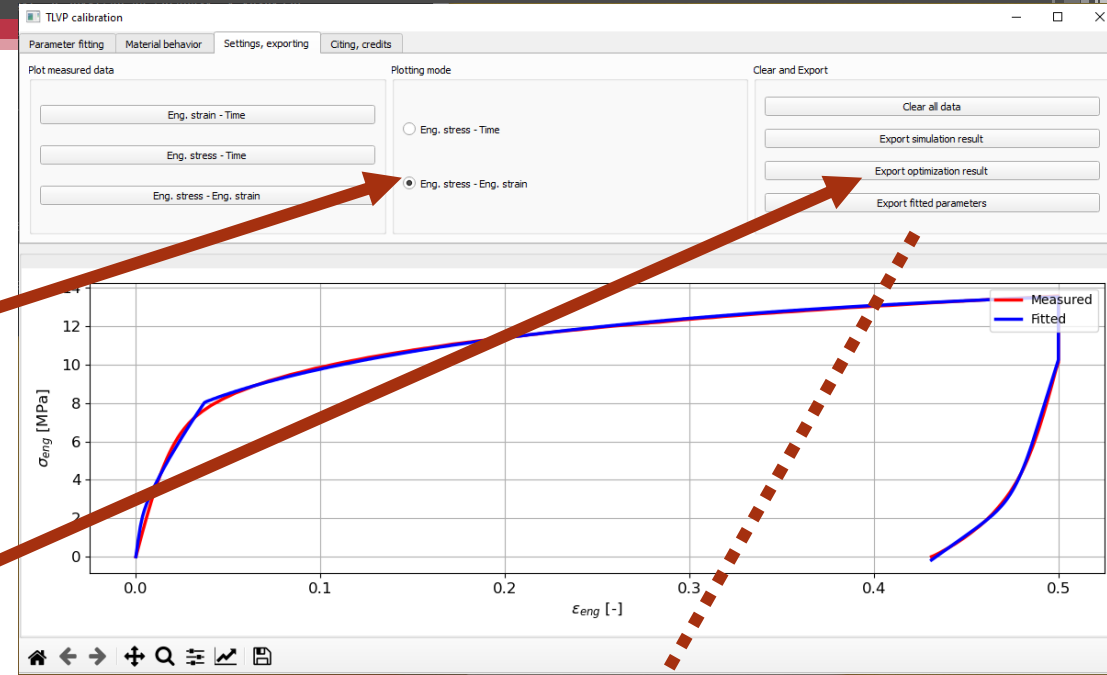
- Did we „hit” any boundaries?
 - No!
 - The plots are quite close too
- The console also has useful information:
 - The optimizer „terminated successfully”, it didn't reach the maxiter or maxfev limit
 - The final value of the normalized squared differences was 0.077
- Conclusion: we are done



```
C:\Users\halev\Documents\bme\phd\paramfitter\tozip\release_v02.exe
Current optimizer parameters: [ 1.2823941  1.15053282  1.67411886  0.78144735  22.33888834  1.19519221
1.83595076]
Current material parameters: [ 7.05316755e+02  8.05372972e-01  5.02235659e+00  3.12578939e+01
4.46777767e-04  3.58557664e+00  -9.17975379e-01]
Current optimizer parameters: [ 1.28284726  1.15038864  1.67522216  0.78116529  22.50628241  1.19401778
1.83580366]
Current material parameters: [ 7.05565993e+02  8.05272048e-01  5.02566649e+00  3.12466117e+01
4.50125648e-04  3.58205334e+00  -9.17901832e-01]
Current optimizer parameters: [ 1.28284726  1.15038864  1.67522216  0.78116529  22.50628241  1.19401778
1.83580366]
Current material parameters: [ 7.05565993e+02  8.05272048e-01  5.02566649e+00  3.12466117e+01
4.50125648e-04  3.58205334e+00  -9.17901832e-01]
None
THREAD COMPLETE!
fun: 0.07765763943134221
jac: array([ 6.53492287e-04, -1.82709843e-03,  4.43316996e-04, -3.12000513e-04,
-3.21809202e-05, -3.78755480e-03,  9.34484415e-04])
message: 'Optimization terminated successfully.'
nfev: 584
nit: 63
njev: 63
status: 0
success: True
x: array([ 1.28284726,  1.15038864,  1.67522216,  0.78116529,  22.50628241,
  1.19401778,  1.83580366])
Number of function evaluations: 584
****FINAL PLOT
Current material parameters: [ 7.05565993e+02  8.05272048e-01  5.02566649e+00  3.12466117e+01
4.50125648e-04  3.58205334e+00  -9.17901832e-01]
```

Plot the srstress-strain curve

- Sometimes the stress-strain graph can give additional insights
- Let's export the results so they can be opened in an other program



The screenshot shows an Excel spreadsheet with the following data:

| #Time [s] | Eng. strain [-] | Measured eng. stress [MPa] | Fitted eng. stress [MPa] |
|----------------------|----------------------|----------------------------|--------------------------|
| 0.000000000000000000 | 0.000000000000000000 | 0.000000000000000000 | 0.000000000000000000 |
| 6.060135060643E-02 | 1.199137538957E-03 | 4.344397641987E-01 | 8.369314428330E-01 |
| 1.212071291228E-01 | 2.418403718208E-03 | 8.70733925801E-01 | 1.572729789573E+00 |
| 1.818180941892E-01 | 3.635003835940E-03 | 1.29961339108E+00 | 2.108134203922E+00 |
| 2.424290400782E-01 | 4.853300877875E-03 | 1.647374938380E+00 | 2.828774660418E+00 |
| 2.92968060449E-01 | 5.85229031946E-03 | 2.062198350057E+00 | 2.76420032754E+00 |
| 3.535721701012E-01 | 7.06367889320E-03 | 2.466351707182E+00 | 3.045219040357E+00 |
| 4.141757351676E-01 | 8.27370275015E-03 | 2.851970471207E+00 | 3.30668862200E+00 |
| 4.747792992240E-01 | 9.49603705032E-03 | 3.202029402311E+00 | 3.560415947070E+00 |
| 5.35372999448E-01 | 1.06907514169E-02 | 3.572257819886E+00 | 3.786931100741E+00 |
| 5.959765647152E-01 | 1.191803788630E-02 | 3.91246682408E+00 | 4.02790669385E+00 |
| 6.56801297817E-01 | 1.31206035224E-02 | 4.231642211379E+00 | 4.284933957804E+00 |
| 7.171836938380E-01 | 1.433437975451E-02 | 4.539087198823E+00 | 4.463368650111E+00 |
| 7.77787258904E-01 | 1.55550797922E-02 | 4.828610651717E+00 | 4.680645278350E+00 |
| 8.38398229607E-01 | 1.674991317274E-02 | 5.09712285109E+00 | 4.878232566320E+00 |
| 8.98994888027E-01 | 1.79784369234E-02 | 5.353384449375E+00 | 5.09510856960E+00 |
| 9.59597958035E-01 | 1.91790023629E-02 | 5.580202559848E+00 | 5.308125339284E+00 |
| 1.020025157150E+00 | 2.038889147400E-02 | 5.81158454179E+00 | 5.49242085324E+00 |
| 1.08005082216E+00 | 2.161466953327E-02 | 6.015904246875E+00 | 5.68916250886E+00 |
| 1.141408846273E+00 | 2.281154100378E-02 | 6.204897060513E+00 | 5.87339670509E+00 |
| 1.202012211199E+00 | 2.40196484888E-02 | 6.383602198149E+00 | 6.07545080211E+00 |
| 1.25296650128E+00 | 2.5043144579178E-02 | 6.5180182197818E+00 | 6.27115847182E+00 |
| 1.313170123195E+00 | 2.62524644249E-02 | 6.671580761667E+00 | 6.41243004430E+00 |
| 1.373773687251E+00 | 2.747654479805E-02 | 6.813561608844E+00 | 6.605374644188E+00 |
| 1.43437725318E+00 | 2.869910612418E-02 | 6.94419831435E+00 | 6.78570654521E+00 |
| 1.494980818374E+00 | 2.989813661031E-02 | 7.062452951567E+00 | 6.96992572121E+00 |
| 1.555484381440E+00 | 3.110004023772E-02 | 7.176624711992E+00 | 7.1424181581E+00 |
| 1.616187946507E+00 | 3.231499631199E-02 | 7.287088592707E+00 | 7.323379316532E+00 |
| 1.676791510563E+00 | 3.353488452971E-02 | 7.37871337206E+00 | 7.50416029162E+00 |
| 1.737395073630E+00 | 3.47011193022E-02 | 7.4692571212E+00 | 7.6892571212E+00 |
| 1.79799619686E+00 | 3.59590424363E-02 | 7.561162611050E+00 | 7.8545565577E+00 |
| 1.858602204752E+00 | 3.715837997531E-02 | 7.640804748378E+00 | 8.01854362974E+00 |
| 1.919205769819E+00 | 3.837909021802E-02 | 7.719210934109E+00 | 8.079198520930E+00 |

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