Steps for GUI

1. Window 1
   Option between
   - Forward modelling
   - Parameter estimation

A. FORWARD MODELLING

INPUT

1. For Forward modelling
   Window 2 (*in_3.dat* file 1st line)
   - nz
   - nm
2. Window 2 (*in_3.dat* file 2nd line)
   - Length (L_e)
   - Bulk density of porous media (ρ_b)
   - Run time (T_{max})
   - Pulse time (T_p)
   - Δt
   - Δx
3. Window 3 (*in_3.dat* file 3rd line)
   - Porosity of the macropore region (θ_f)
   - Porosity of the mesopore region (θ_s)
   - Porosity of the micropore region (θ_{im})
4. Window 4 (*in_3.dat* file 4th line)
   - Instantaneous sorption fraction in macropore region (F_f)
   - Instantaneous sorption fraction in mesopore region (F_s)
   - Instantaneous sorption fraction in micropore region (F_{im})
   - Fraction of sorption site available for macropore region (f_f)
   - Fraction of sorption site available for mesopore region (f_s)
   - Fraction of sorption site available for immobile region (f_{im})
5. Window 4 (*in_3.dat* file 5th line)
   - Equilibrium sorption coefficient in macropore region (K_f)
   - Equilibrium sorption coefficient in mesopore region (K_s)
   - Equilibrium sorption coefficient in micropore region (K_{im})
   - Rate-limited sorbed coefficient in macropore region (k_f)
   - Rate-limited sorbed coefficient in mesopore region (k_s)
   - Rate-limited sorbed coefficient in micropore region (k_{im})
6. Window 5 (*in_1.dat* file)
   - Mesopore seepage velocity (q_s)
   - Macropore seepage velocity (q_f)
   - Solute mass transfer rate b/w meso-micropore (ω_{im})
   - Solute mass transfer rate b/w meso-macropore (ω_{sf})

- Dispersivity (α_L)
- No. of observation time steps
- Experimental data (%Input from txt file or excel copy paste)

7. Window 6 (*in_2.dat* file)
    - No. of observation distances to print
    - Observation distances (% according to No.of observation distances)
    - Time steps (%Input from txt file or excel copy paste)
8. Run *test.exe*

OUTPUT

1. Read *OUTPUT.dat* here first column is experimental data and rest is simulated data at different distances. (Concentrations)
2. Read No. of observation time steps from *IN_2.dat* (Time)
3. Plot Concentration vs time graph for different distances with option to display one at a time to all at a time

B. PARAMETER ESTIMATION

INPUT

Same steps until pt. 6

1. Window 5 (*in_1.dat* file)
    - Mesopore seepage velocity (q_s) [checkbox for Determined or Initial guess]
    - Macropore seepage velocity (q_f) [checkbox for Determined or Initial guess]
    - Solute mass transfer rate b/w meso-micropore (ω_{im}) [checkbox for Determined or Initial guess]
    - Solute mass transfer rate b/w meso-macropore (ω_{sf}) [checkbox for Determined or Initial guess]
    - Dispersivity (α_L) [checkbox for Determined or Initial guess]
    - No. of observation time steps
    - Experimental data (%Input from txt file or excel copy paste)
2. Window 6 (*in_2.dat* file)
    - No. of observation distances to print
    - Observation distances (% according to No.of observation distances)
    - Time steps (%Input from txt file or excel copy paste)
3. Run *test.exe*
4. Save as *in_1.dat* file as *in_1.tpl* as

```
ptf #
#qs          #
0.4
#omegaim     #
#omegasf     #
#alpha       #
43
0.006706908
0.046277666
0.075117371
0.117370892
0.153588196
```

Changes to be made:-

- First line write [ptf #]
- Parameters which are to be estimated should come in between ## e.g. [# qs #]
- Parameter determined will remain with the same values given before e.g.[qf = 0.4]

5. Run *tempchek in_1.tpl* in command prompt
6. Create *in_1.par* such as

```
single point
 qs  0.2641   1.0   0.0
 omegaim  0.000047   1.0   0.0
 omegasf  0.00976    1.0   0.0
 alpha  0.52  1.0   0.0
```

Here

- first character is name of the parameter
- second is the initial guess supplied
- next 1 and 0 are default

7. Run *tempchek in_1.tpl in_1.dat in_1.par* in command prompt
8. Write a file *output.ins* such as

```
pif #
l1 (o1)19:26
l1 (o2)19:26
l1 (o3)19:26
l1 (o4)19:26
l1 (o5)19:26
l1 (o6)19:26
l1 (o7)19:26
l1 (o8)19:26
```

Here

- (o1) is the observation point and it should go up to max. observation time steps
- Rest will remain same for each line

9. Run *inschek output.ins* in command prompt
10. Run *inschek output.ins output.dat*
11. Save experimental data from *in_1.dat* in *measure.obf* corresponding to observation number

```
o1      0.006706908
o2      0.046277666
o3      0.075117371
o4      0.117370892
o5      0.153588196
o6      0.174379611
o7      0.210596915
o8      0.240107311
o9      0.26425218
```

12. Run *pestgen test in_1.par measure.obf* (It will generate *test.tpl* file)

13. Window 7 (edit *test.tpl* file)

```
* parameter data
qsl          none relative  0.200      1.000000E-10  1.000000E+10 qsl          1.0000     0.0000     1
alphaim      none relative  4.700000E-02 1.000000E-10  1.000000E+10 alphaim      1.0000     0.0000     1
alphasf      none relative  6.760000E-03 1.000000E-10  1.000000E+10 alphasf      1.0000     0.0000     1
alpha        none relative  0.20000    1.000000E-10  1.000000E+10 alpha        1.0000     0.0000     1
```

- Ask for Lower Bound and Upper Bound for the estimating parameters
- Insert values of lower bound in place of Blue highlighted and upper bound in place of yellow highlighted area corresponding to parameters.
- Edit highlighted part of *test.tpl*

```
* model command line
model
* model input/output
model.tpl       model.inp
model.ins       model.out
* prior information
```

into

```
* model command line
test
* model input/output
in_1.tpl        in_1.dat
output.ins      output.dat
* prior information
```

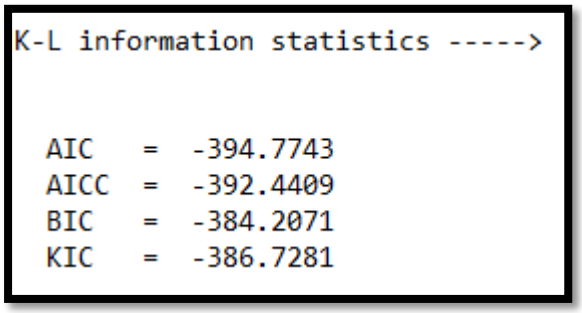
14. Run *pestchek test*
15. Run *pest test* (It generates *test.rec* file)

OUTPUT

1. Display table from *test.rec*

Parameter	Estimated value	95% percent confidence limits lower limit	upper limit
qsl	0.293725	0.288016	0.299434
qfs	0.388452	0.375032	0.401873
alphaim	1.000000E-10	-11534.3	11534.3
alphasf	6.139572E-03	4.165871E-03	8.113274E-03
alpha	0.366416	0.287786	0.445046

2. Display table from *test.rec*



3. Read *OUTPUT.dat* here first column is experimental data and rest is simulated data at different distances. (Concentrations)
4. Read No. of observation time steps from *IN_2.dat* (Time)
5. Plot Concentration vs time graph for different distances with option to display one at a time to all at a time