Kintecus GUI

User Guide

Web-based interface for the Kintecus chemical kinetics simulator

Version 1.0 · May 2026

Contents

1. Getting Started

Kintecus GUI is a web-based replacement for the Excel-VBA front end that has traditionally been used to drive the Kintecus chemical kinetics simulator. It runs entirely on your own machine — the "web server" is a small Python program that listens only on localhost (127.0.0.1) and opens a browser tab automatically. This GUI does NOT require any form of Office or Excel.

Installing

The installer Kintecus_GUI_Setup.exe assumes the main Kintecus package has already been installed (**kintecus.exe** must exist at the chosen install directory, normally C:\Kintecus\). The installer will refuse to proceed if kintecus.exe is missing — that is your cue to install or repair the main package first.

After installation:

- A Start Menu shortcut "Kintecus GUI" launches the GUI.
- An optional desktop shortcut can be created during installation.
- Any .kintpack file becomes double-clickable — Windows will open it with kintecus_gui.exe automatically.

Launching

Start kintecus_gui.exe (or double-click any .kintpack file). A console window appears showing log output, and after about two seconds your default browser opens to http://localhost:5000.

Command-line flags:

```
kintecus_gui.exe                                (start GUI with empty state)
kintecus_gui.exe --help                         (show available flags and exit)
kintecus_gui.exe -kintpack MyProject.kintpack (auto-load a saved package)
```

Layout of the Interface

Every page shares the same layout:

- Top header — the green dot confirms the local server is alive.
- Left sidebar — navigation between the eleven pages.
- Main panel area — page-specific controls and grids.

2. Home Page & .kintpack Packages

The Home page is dedicated to project management. A .kintpack file is a single-file JSON snapshot of your entire project: every grid (Model, Species, Parameters, Thermodynamics, Fit Data, all O_ files), every setting, and your free-form description.

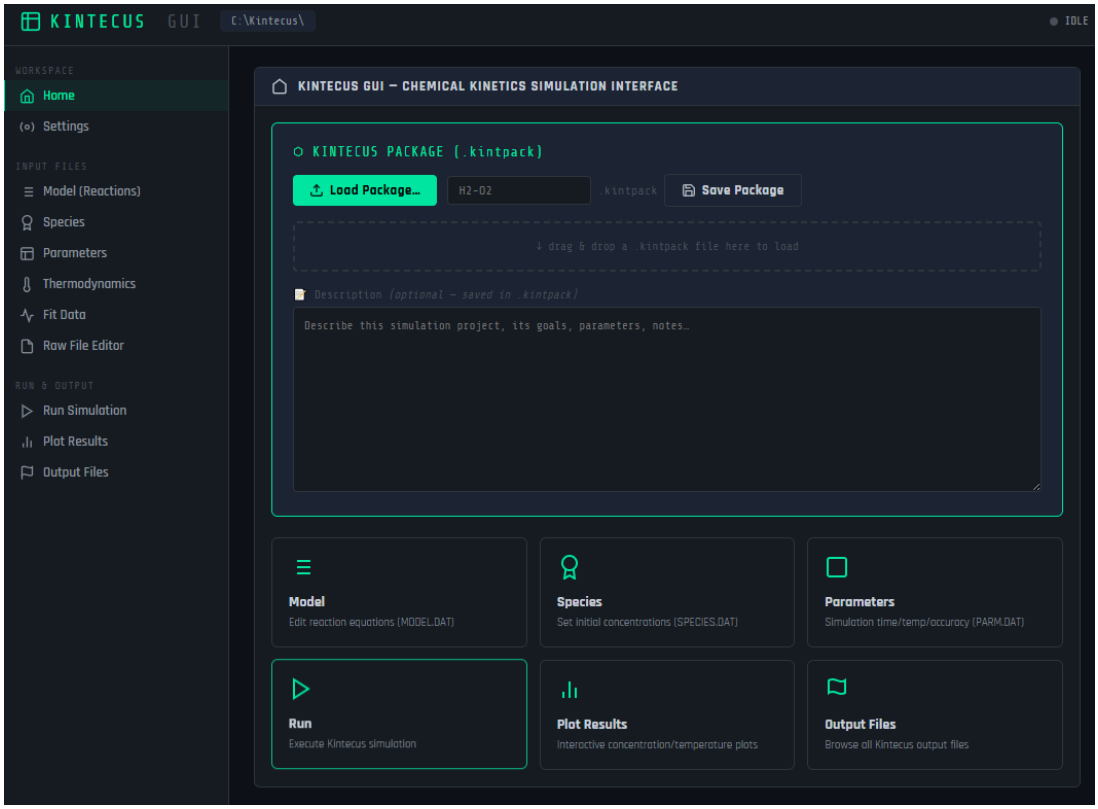


Figure 1. The Home page — Save / Load .kintpack packages and the optional description box.

Saving a Package

1. Type a short name in the package-name box (e.g. "H2-O2" or "Enzyme_Regression"). The .kintpack extension is added automatically.
2. Optionally type a free-form description in the large text areabox — this is stored inside the .kintpack file and restored when you load it.
3. Click 💾 Save Package — your browser downloads <name>.kintpack to its normal download location.

Loading a Package

There are three ways to load a package:

- Click 📂 Load Package… and pick a .kintpack file.
- Drag a .kintpack file from your desktop onto the dashed drop-zone.
- Double-click a .kintpack file in Windows Explorer — the GUI launches and auto-loads it.

What Gets Saved

Everything you would lose if you closed the browser. The save covers:

- Settings (Kintecus path, default switches, locale, Kintecus key).
- All editable grids: Model, Species, Parameters, Thermodynamics, Fit Data.
- All O_ perturbation/fit-data files (filename, columns, every cell).
- The description text.
- Your output files from a Kintecus run, such as concentrations (CONC.TXT), optimized/regressed values (OPTOUT.TXT), NSA files, or anything Kintecus creates are **NOT SAVED** with the Kintpack file. You have to manually copy or rename those!

3. Settings

The Settings page configures the Kintecus environment and persistence options. Most users only need to set the Kintecus Path once. Note that these settings from a Kintecus-Excel model, and are stored on the CONTROL worksheet.

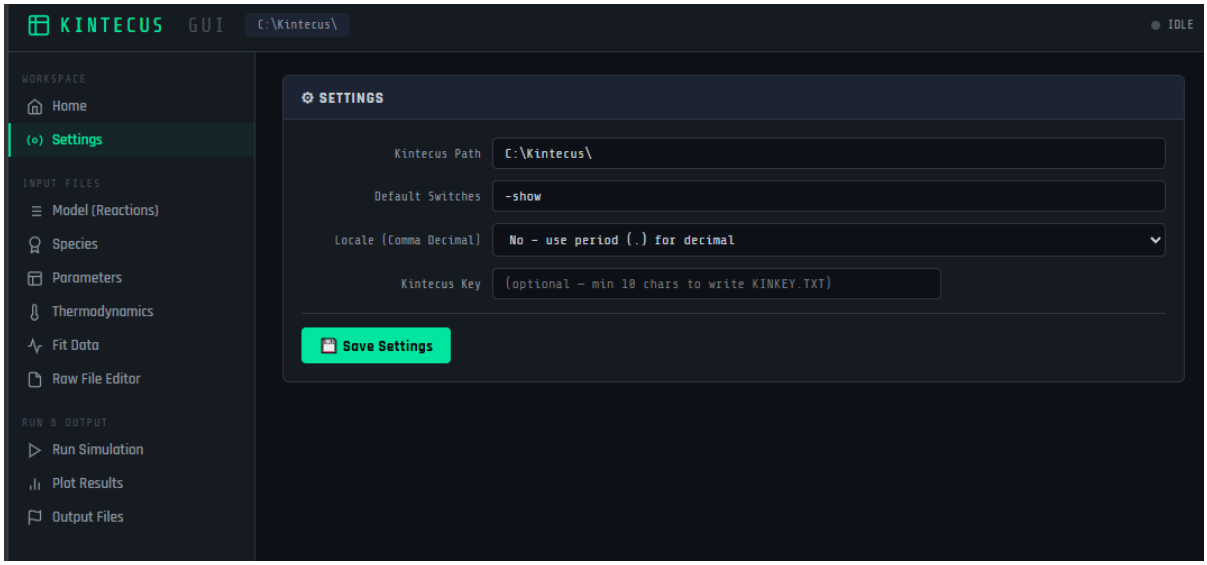


Figure 2. Settings page — Kintecus path, default switches, locale, and Kintecus key.

Field	Purpose
Kintecus Path	Directory containing kintecus.exe and the working data files (default C:\Kintecus\). All DAT files and TXT output land here.
Default Switches	Switch line that pre-populates the Run Simulation page. Common examples: -show -INT:5 -CONF -CHEMNET
Locale	Set to "Yes" only if your spreadsheet exports use comma as the decimal separator (German/France locales). The default "No" keeps the standard period.
Kintecus Key	Optional license key. If at least 10 characters are entered, the value is written to KINKEY.TXT at the start of every Run Kintecus.

Click 💾 Save Settings to persist the values to disk so they survive a GUI restart.

4. Model Page — Reactions

The Model page is where your reaction mechanism lives. Each row is one reaction expressed in Kintecus syntax. The five columns map directly to the columns of MODEL.DAT. Note that these settings from a Kintecus-Excel model, are stored on the MODEL worksheet. If you have a Kintecus-Excel Worksheet, and if you click “RUN” on the CONTROL, the “MODEL.DAT” file is saved and can easily be directly loaded here in this GUI by clicking “Load MODEL.DAT”.

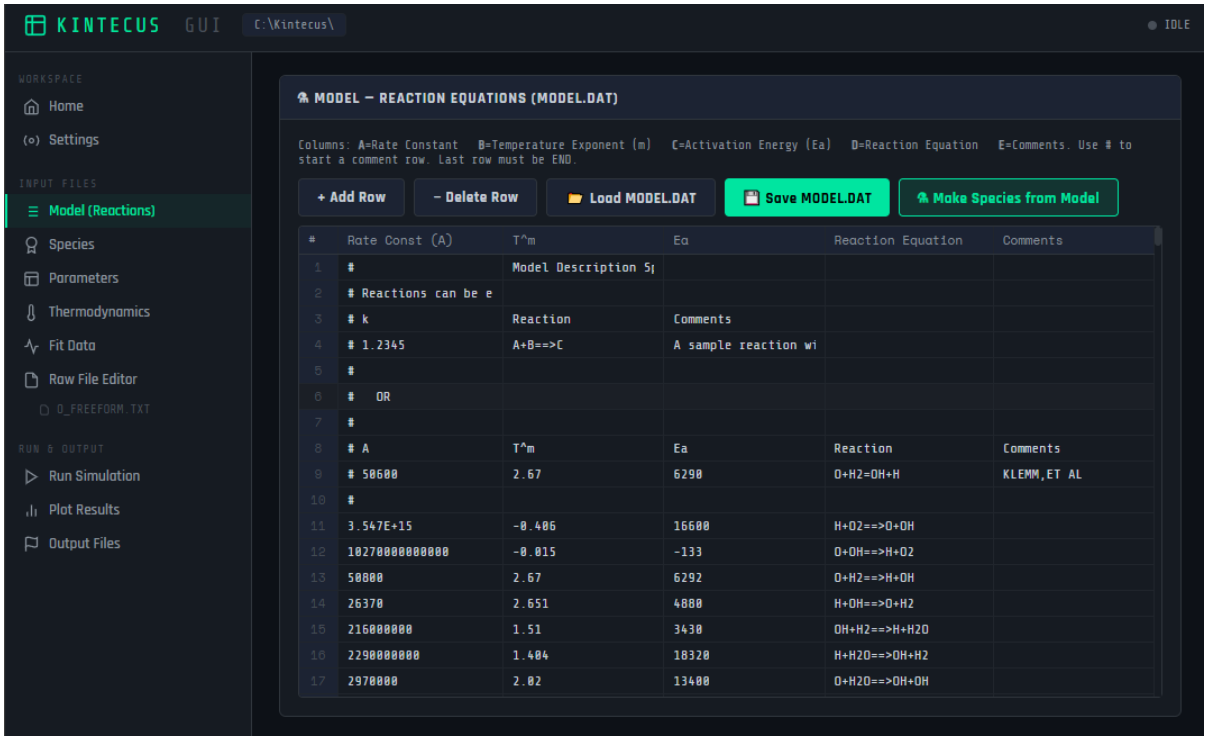


Figure 3. Model page — reactions with Arrhenius parameters and rate-constant comments.

Column	Meaning
A — Reaction	The reaction itself in Kintecus syntax, e.g. H2+OH=H+H2O.
B — A factor	Pre-exponential factor of the modified Arrhenius expression.
C — n	Temperature exponent.
D — Ea	Activation energy. Units are set by the PARM grid (KCAL, KJOULES, etc.).
E — comment	Free-form comment column. Ignored by Kintecus.

Row controls

- + Add Row inserts a blank row after the currently-focused row (click in a cell first to set focus). At the end of the list, it appends.
- − Delete Row removes the focused row. A minimum of 2 rows is enforced.
- 📂 Load MODEL.DAT loads an existing MODEL.DAT file into the grid.

- The last row of any model must contain "END" in column A — this is added automatically when the grid is first populated.

Make Species from Model

Click ⚗ Make Species from Model and confirm — the GUI will:

1. Write the current Model grid to MODEL.DAT.
2. Run kintecus.exe -c -i, which parses the reactions and builds a fresh SPECIES.DAT plus ADDSPEC.TXT.
3. Load the result into the Species grid and navigate you to that page.

This is the fastest way to bootstrap a Species grid for a brand-new mechanism. It overwrites the existing Species grid completely, so use with care.

5. Species Page

The Species page lists every chemical species participating in your model, along with starting conditions and display options. Each row becomes one line of SPECIES.DAT. Note that these settings are from a Kintecus-Excel workbook and are stored on the SPECIES worksheet. If you have a Kintecus-Excel Worksheet, if you click “RUN” on the CONTROL worksheet, the “SPECIES.DAT” file is saved and can easily be directly loaded here in this GUI by clicking “Load SPECIES.DAT”.

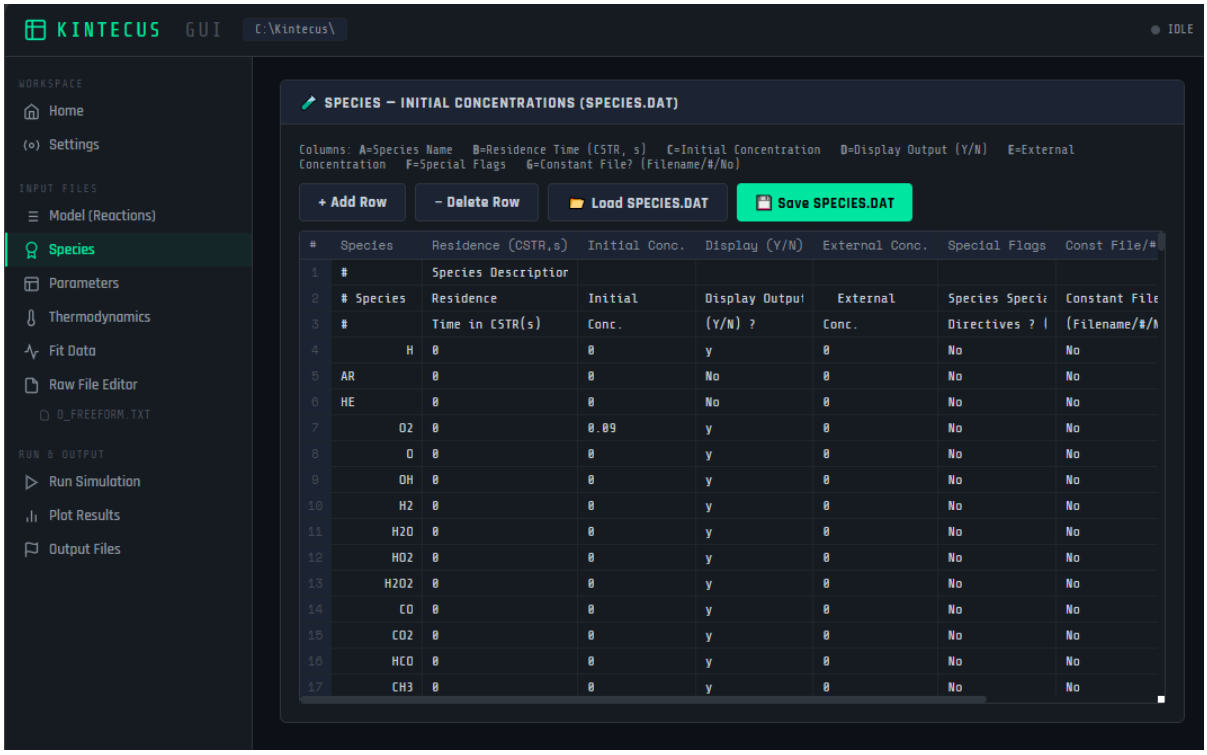


Figure 4. Species page — concentrations, display flags, and special-handling options for each species.

Column	Meaning
Species	Species name (must match exactly what appears in the Model reactions).
Residence	Residence time for flow-reactor calculations. 0 for batch.
InitConc	Initial concentration at t=0.
Display	Yes / No — whether this species appears in the main concentration plot.
ExtConc	External-concentration filename (when using imposed-concentration profiles).
Special Flags	Flags for special-handling (see manual for further details).
ConstFile	Filename for time-varying parameters perturbations, if any.

6. Parameters Page

The Parameters page (PARM.DAT) controls the integrator behavior, temperature/pressure profile, constant pressure run, units and other parameters at startup. Each row contains five generic columns A–E whose meaning depends on the row number. This intentionally mirrors how Kintecus parses PARM.DAT. Note that these settings are from a Kintecus-Excel workbook and are stored on the PARM worksheet. If you have a Kintecus-Excel Worksheet, and if you click “RUN” on the CONTROL worksheet, the “PARM.DAT” file is saved and can easily be directly loaded here in this GUI by clicking “Load PARM.DAT”.

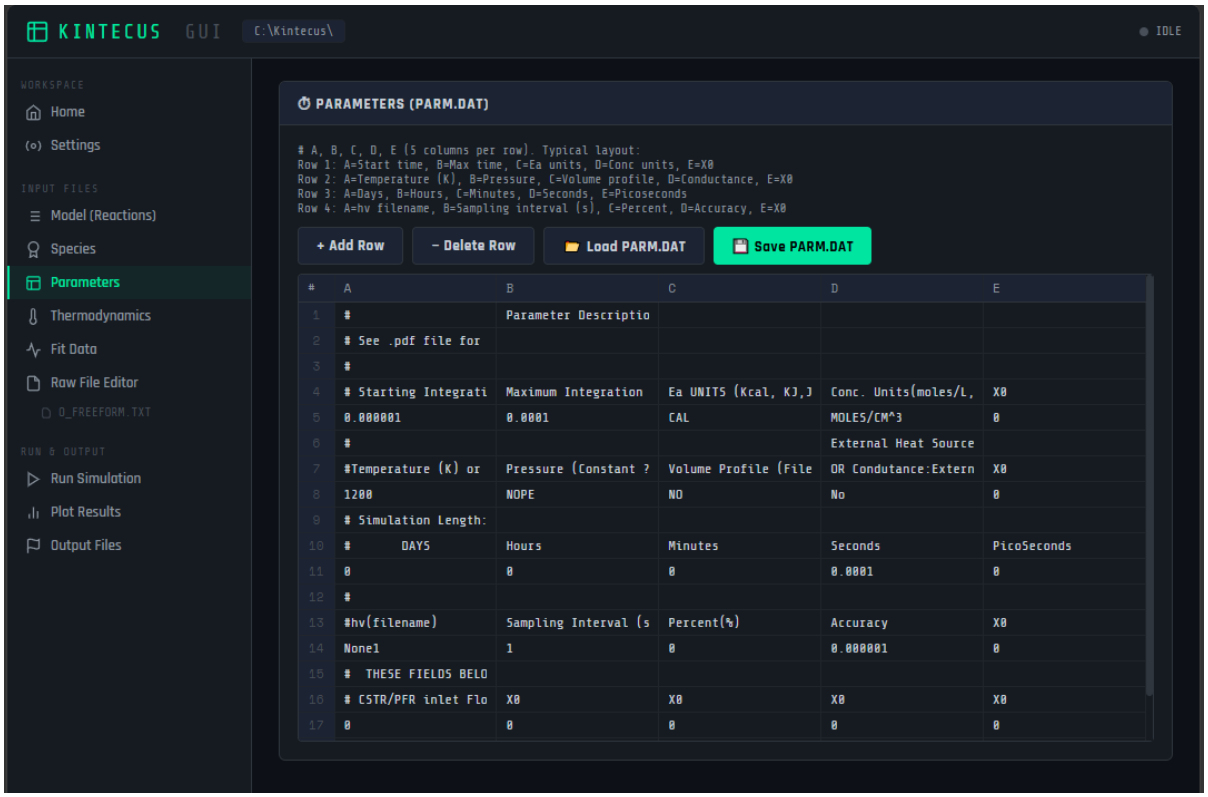


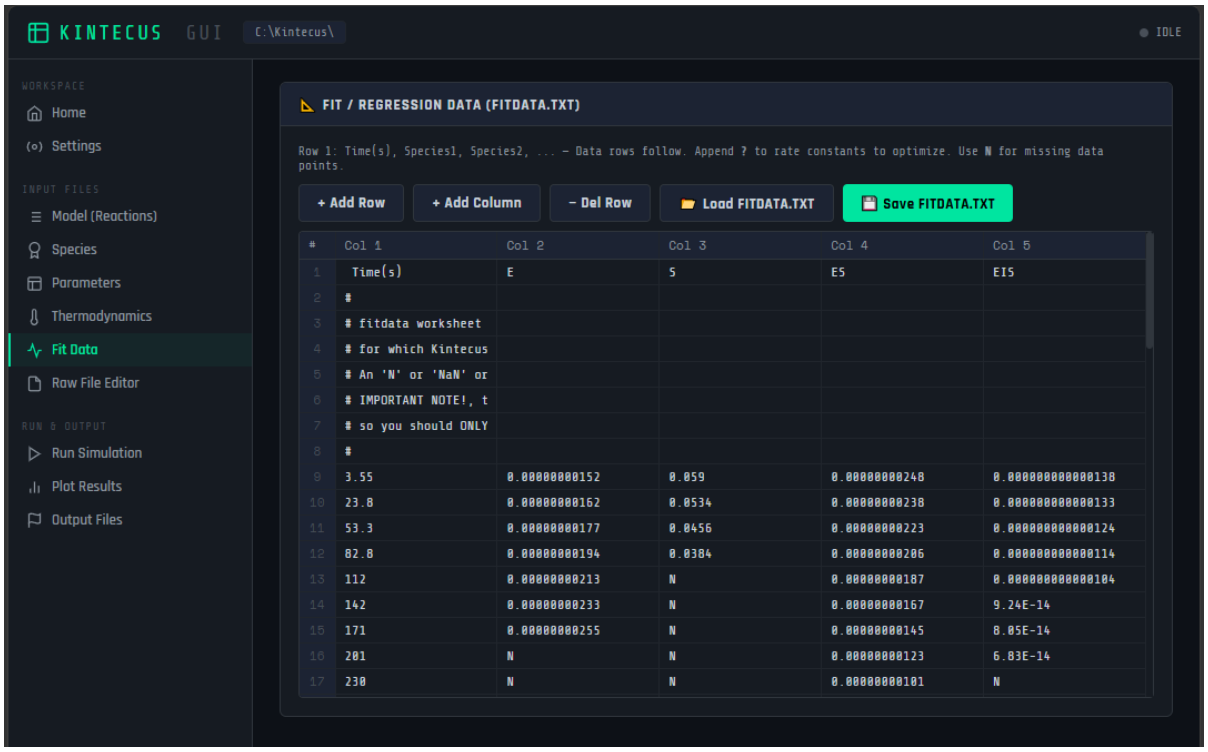
Figure 5. Parameters page — five generic columns (A–E) whose meaning depends on row number.

Row	A, B, C, D, E
1	Start time, Max time, Ea units, Conc units, X0
2	Temperature(K), Pressure, Volume profile, Conductance, X0
3	Days, Hours, Minutes, Seconds, Picoseconds
4	hv filename, Sampling interval (s), Percent, Accuracy, X0

Refer to the Kintecus manual for the full list of acceptable values in each cell. The grid mirrors the PARM worksheet from the original Excel/VBA workflow row-for-row.

7. Thermodynamics Page

The Thermodynamics page holds a description of the thermodynamic parameters used in your model. Please see Kintecus Manual for a full description. The example in the figure below shows that this run will utilized thermodynamic values for a file named “freeform.txt”. That file is stored inside a kintpack as an “O_” file in the “Raw File Editor” . Note that these settings are from a Kintecus-Excel workbook and are stored on the optional THERM worksheet. If you have a Kintecus-Excel Worksheet, and if you click “RUN” on the CONTROL worksheet, the “THERM” worksheet is saved and can easily be directly loaded here in this GUI by clicking “Load THERM.DAT”. You’ll also need to load the “FREEFORM.TXT” file into the “Raw File Editor” part by clicking it and click “ADD FILE” in that part.



#	Col 1	Col 2	Col 3	Col 4	Col 5
1	Time(s)	E	5	E5	E15
2	#				
3	# fitdata worksheet				
4	# for which Kintecus				
5	# An 'N' or 'NaN' or				
6	# IMPORTANT NOTE!, t				
7	# so you should ONLY				
8	#				
9	3.55	0.00000000152	0.059	0.00000000248	0.0000000000000138
10	23.8	0.00000000162	0.0534	0.00000000238	0.0000000000000133
11	53.3	0.00000000177	0.0456	0.00000000223	0.0000000000000124
12	82.8	0.00000000194	0.0384	0.00000000206	0.0000000000000114
13	112	0.00000000213	N	0.00000000187	0.0000000000000104
14	142	0.00000000233	N	0.00000000167	9.24E-14
15	171	0.00000000255	N	0.00000000145	8.05E-14
16	201	N	N	0.00000000123	6.83E-14
17	230	N	N	0.00000000101	N

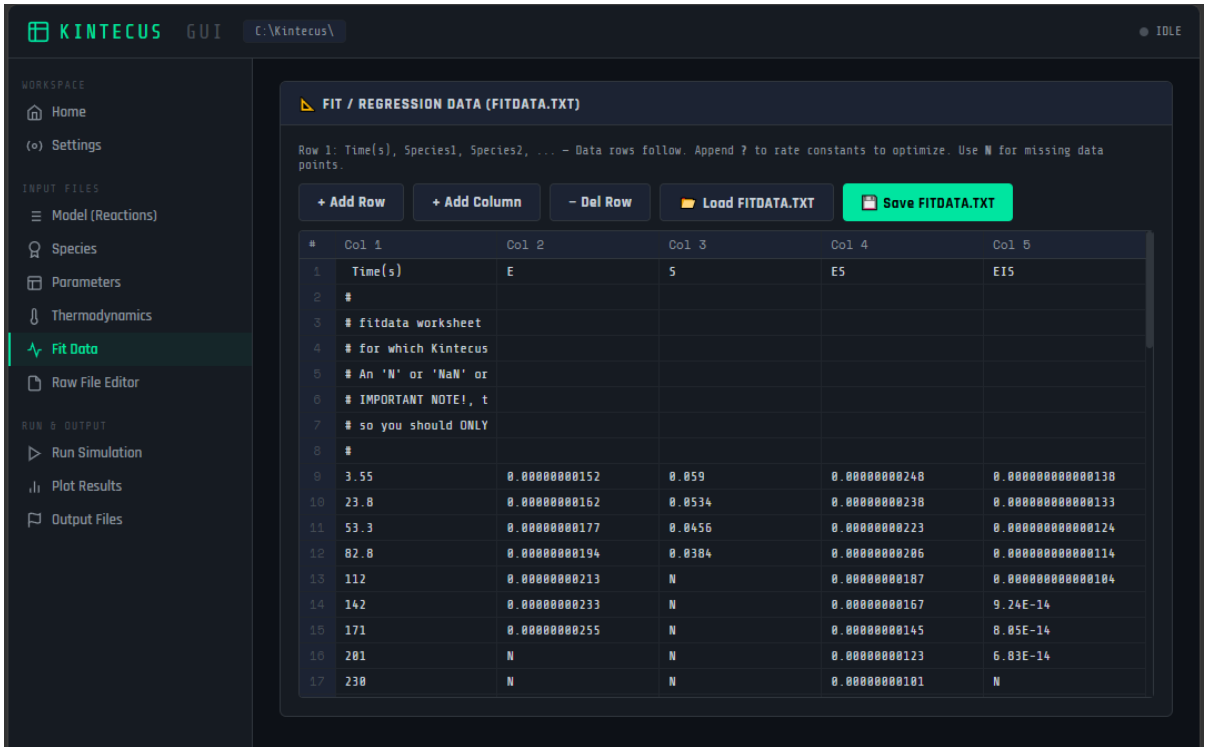
Figure 6. Fit Data page — experimental data with one column per species and N for missing values.

- Column 1 is always Time(s).
- Each subsequent column corresponds to a species — the column header must match the species name exactly.
- Missing values are written as "N", "NaN", or "None" — Kintecus skips these points during the fit.
- The last row must contain "END" in column 1.
- Load an existing FITDATA.TXT file with 📂 Load FITDATA.TXT, or build the grid by hand.

For multi-fit runs (-FIT: with :FITDATAN switch), use the Raw File Editor to add multiple FITDATAN.TXT files as O_ files — see the next section.

8. Fit Data Page

The Fit Data page holds your experimental data — the targets that Kintecus will fit rate constants against when the -FIT flag is on the command line. Note that these settings are from a Kintecus-Excel workbook and are stored on the optional FITDATA worksheet. If you have a Kintecus-Excel Worksheet, and if you click “RUN” on the CONTROL worksheet, the “FITDATA.TXT” file is saved and can easily be directly loaded here in this GUI by clicking “Load FITDATA.TXT”.



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- Load an existing FITDATA.TXT file with 📂 Load FITDATA.TXT, or build the grid by hand.

For multi-fit runs (-FIT: with :FITDATAN switch), use the Raw File Editor to add multiple FITDATAN.TXT files as O_ files — see the next section.

9. Raw File Editor & O_ Files

The Raw File Editor has two distinct sections and tries to mimic the behavior of “O_” worksheets in the Kintecus-Excel workbooks.

Raw File Editor (top section)

A plain text-area for editing any file in the Kintecus directory by name. Type the filename (e.g. CONC.TXT) and click 📂 Load to read it, or 💾 Save to write the current text contents back.

O_ Perturbation / Fit-Data Files (bottom section)

This section is the equivalent of all the O_<something> worksheets in the original Excel workbook. Up to 99 O_ files can be active at once. When you click Run Kintecus, each O_ file is written to the Kintecus directory with the "O_" prefix stripped from its name — so an O_FITDATA1.TXT entry in the GUI becomes FITDATA1.TXT on disk.

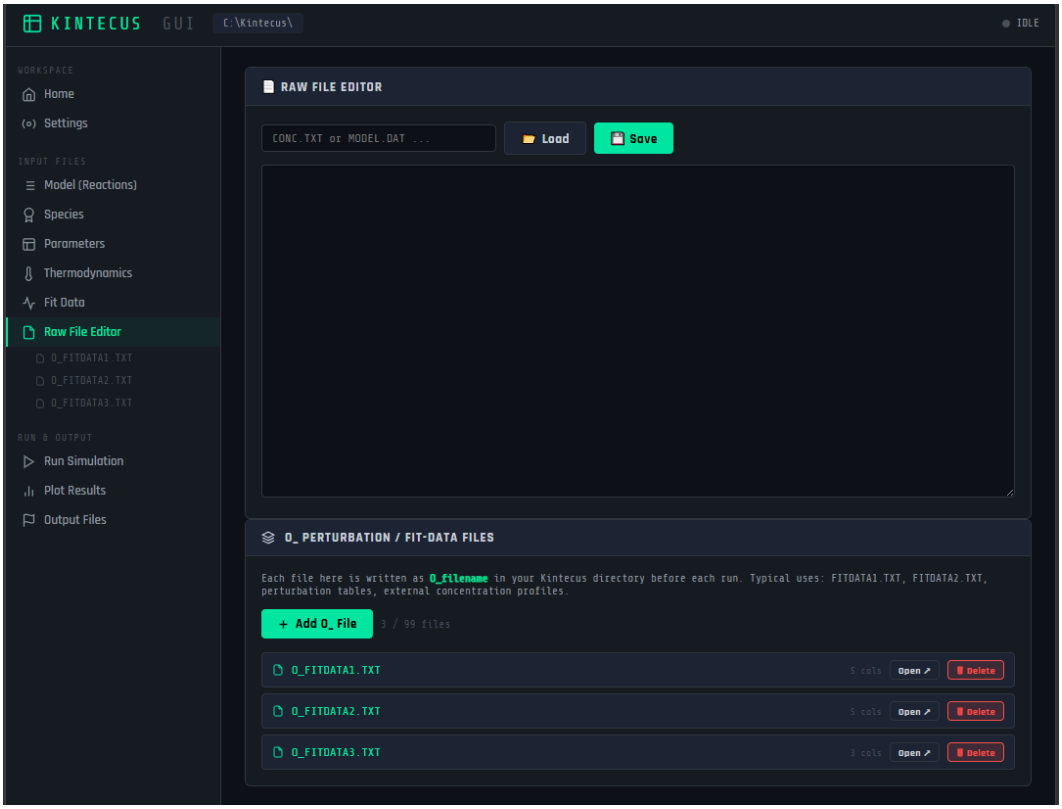

Figure 7. Raw File Editor with three O_ perturbation/fit-data files loaded.

Adding O_ files

Click + Add O_ File and pick a tab-delimited .txt, .dat, or .csv file. The GUI:

1. Adopts the file's name as the entry name (uppercased).
2. Adds a new sub-item to the sidebar under "Raw File Editor".

3. Opens the file in a full-grid editor with column headers detected from the first row if it looks like a header.
4. Navigates to the new grid page so you can verify it.

Editing O_ files

Each O_ grid has +/− Add/Delete Row, + Add Column, 📂 Load File…, 💾 Save to Kintecus dir, and 🗑 Delete This O_ File buttons. The grid behaves identically to the other grids.

Deleting O_ files

Either click the 🗑 Delete next to a file in the summary list on the Raw File Editor page, or 🗑 Delete This O_ File from the file's own grid page. A confirmation is required.

10. Run Simulation

The Run Simulation page is where you actually launch Kintecus. The page shows a live log of standard output and a row of "View" / "Plot" buttons that dynamically appear based on which switches you have on the command line.

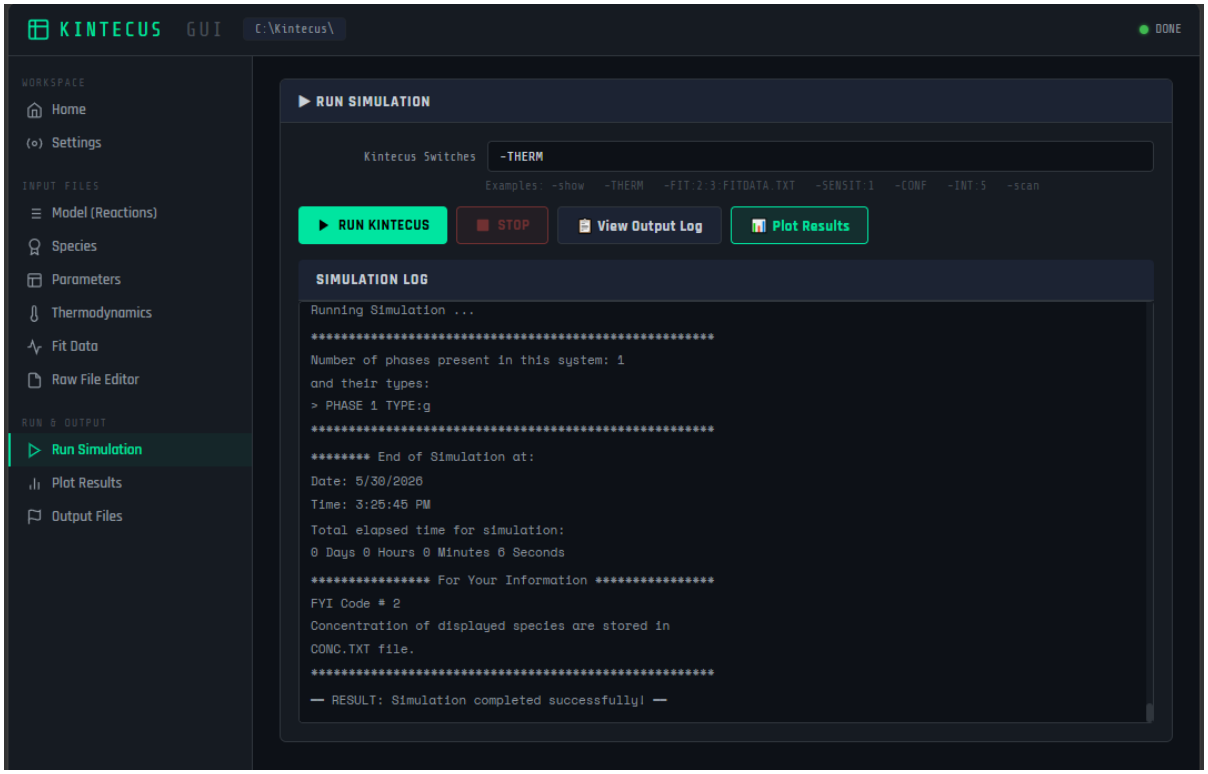

Figure 8. Run Simulation page — switches field, live log, and contextual View / Plot buttons.

The Switches Field

Pre-populated from Settings, but you can edit it for one-off runs. Some common switches:

Switch	Effect
-show	Display Kintecus banner and progress text.
-INT:N	Select type of integrator (1-5)
-FIT	Single-file fitting mode using FITDATA.TXT.
-FIT:start:end:FITDATAN	Multi-file fitting mode (uses FITDATA1.TXT, FITDATA2.TXT…).
-CONF	Confidence/Monte-Carlo analysis (produces CONCAVG, CONCSTD, CONCMAX, CONCMIN).
-SENSIT	Sensitivity analysis (produces SENSITnnn.TXT files).
-scan	Parameter-scan run (produces CONCnnnnnn.TXT files).

-CHEMNET	Generate chemnetwork.png chemical-network diagram.
-THERM	Include thermodynamic outputs.

Mutually exclusive switches

Important: -SCAN, -SENSIT, -FIT, and -CONF are mutually exclusive. If you accidentally combine any two, both Run Kintecus and Plot Results will refuse to proceed and tell you exactly which flags are in conflict.

Running

Click ▶ RUN KINTECUS. The button disables, the status dot turns yellow (RUNNING), and the live log fills in as Kintecus writes to standard output. Pressing ■ STOP terminates the subprocess cleanly.

When the run completes

- Status dot turns green DONE on success, yellow WARNINGS if KWARN.OUT was produced, red ERROR if KERR.OUT was produced or KDONE.OUT contains "FATAL".
- On a fatal error the GUI pops up the KDONE.OUT message and offers to open the tail of view.txt so you can find the cause.
- If -CHEMNET was active, the chemnetwork image pops up automatically.

Contextual View / Plot buttons

- 📋 View Output Log — opens view.txt (every line Kintecus printed).
- 📋 View Fit Results — appears only when -FIT is in switches. Opens OPTOUT.TXT.
- 🔬 View Chemnet — appears only when -CHEMNET is in switches. Opens the chemnetwork image.
- 📊 Plot Results — navigates to the Plot Results page (always present).

11. Plot Results

The Plot Results page is the rich visualization hub. It contains a main concentration chart at the top and then up to four additional analysis panels that appear or disappear based on which switches you ran with. The page is fully rebuilt every time you navigate to it or load a kintpack, so it always reflects the current switches.

10a. Main Concentration Plot

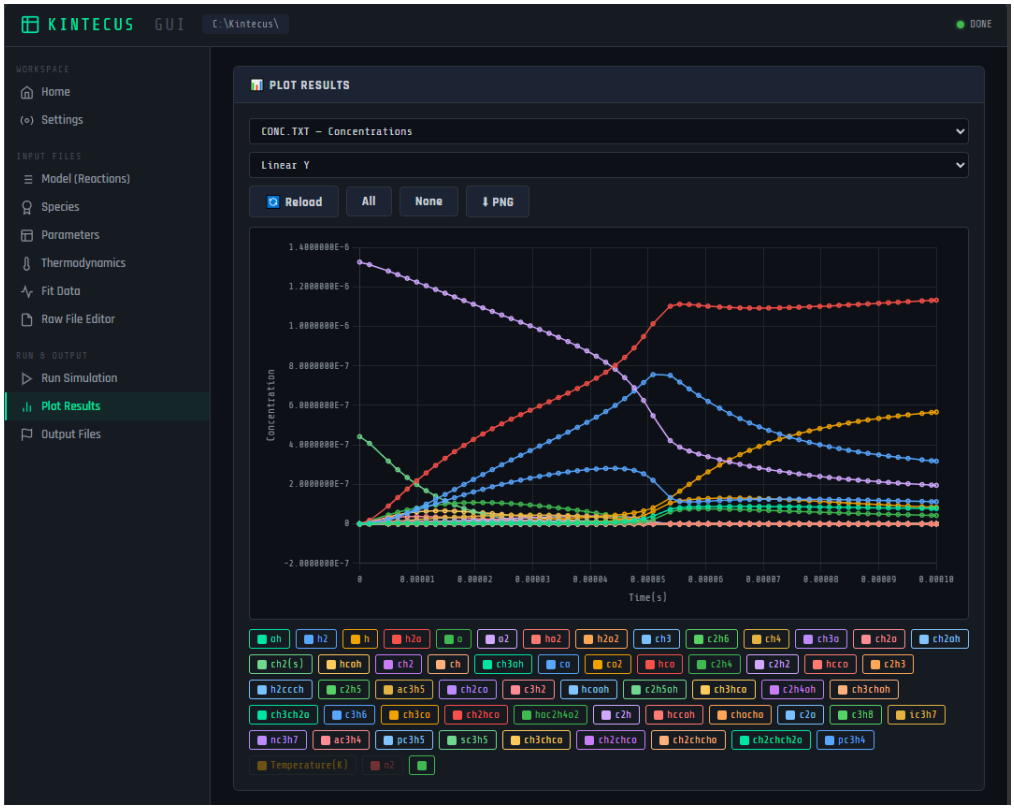

Figure 9. Main chart — concentrations from CONC.TXT (or other selectable Kintecus output files).

- The file dropdown is populated dynamically. CONC.TXT is always available; RATESOUT/SPECRATE/THERMOUT appear with -o:, CONCAVG/CONCMAX/CONCMIN with -CONF, OPTOUT.TXT with -FIT, SCANS.TXT with -scan.
- Linear or Logarithmic Y-axis via the second dropdown.
- 🔄 Reload re-reads the file from disk.
- All / None toggle every species at once. Individual species can be toggled by clicking their pill underneath the chart.
- ⇩ PNG saves the current chart as a PNG image.

11b. Experimental vs. Fitted Data

Appears only when -FIT is in the switches. Implements the DoFitPlot logic from the original VBA: simulated concentrations as lines, experimental data points as open circles in the matching color.

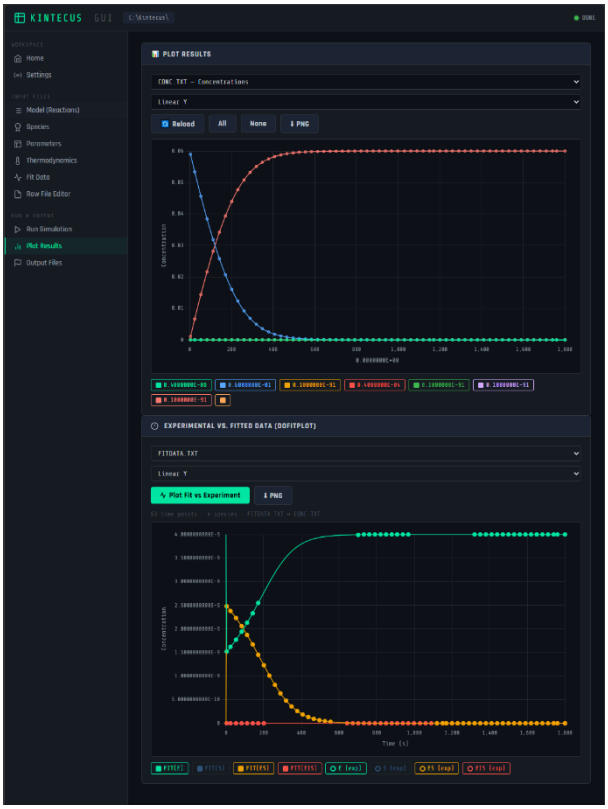

Figure 10. Fit comparison — simulated curve (line) overlaid with experimental data (circles).

- For single-FIT runs the dropdown shows only FITDATA.TXT. For multi-FIT runs (with :FITDATAN in switches) it lists every numbered FITDATA1.TXT, FITDATA2.TXT… file found on disk.
- Each numbered FITDATA<n>.TXT is paired with its matching CONC<n>.TXT.
- Experimental points marked "N" are skipped (no dot drawn).
- The status line confirms the paired files, e.g. "52 time points · 4 species · FITDATA1.TXT ↔ CONC1.TXT".

11c. Sensitivity (NSC) Heatmaps

Appears only when -SENSIT is in the switches. Renders each SENSITnnn.TXT file as a 2D heatmap.

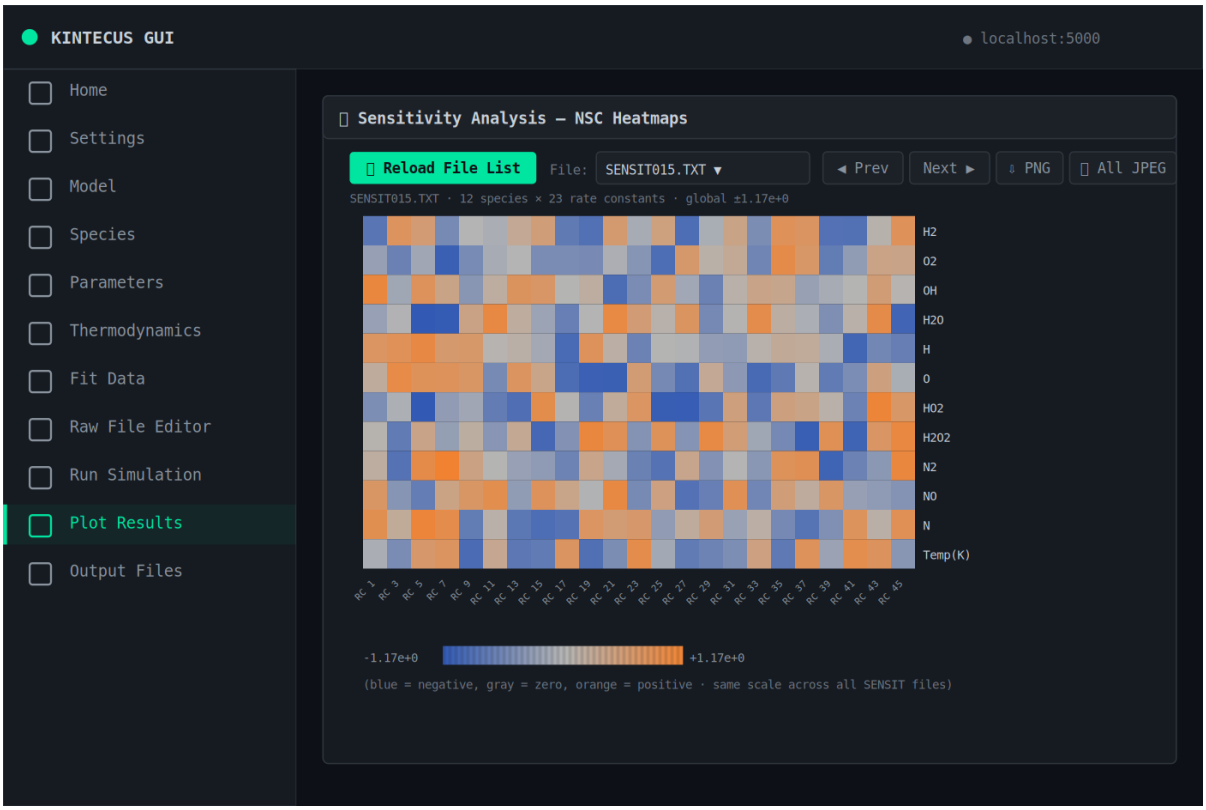

Figure 11. Sensitivity heatmap — species (rows) × rate constants (columns) with diverging blue / gray / orange palette.

- When the panel loads, all SENSIT files are scanned to determine a global color scale (99th-percentile based, so a single outlier won't wash out everything else).
- The same color scale is used for every file so heatmaps are directly comparable across time points.
- ◀ Prev / Next ▶ step through the SENSITnnn.TXT files in numerical order. The dropdown jumps directly.
- ⇩ PNG saves the current heatmap. Export All as JPEG saves every SENSITnnn.TXT as a JPEG in one click.
- Color key: blue = negative NSC, gray = zero, orange = positive NSC.

11d. Confidence Analysis (CONF)

Appears only when -CONF is in the switches. Three views are available:

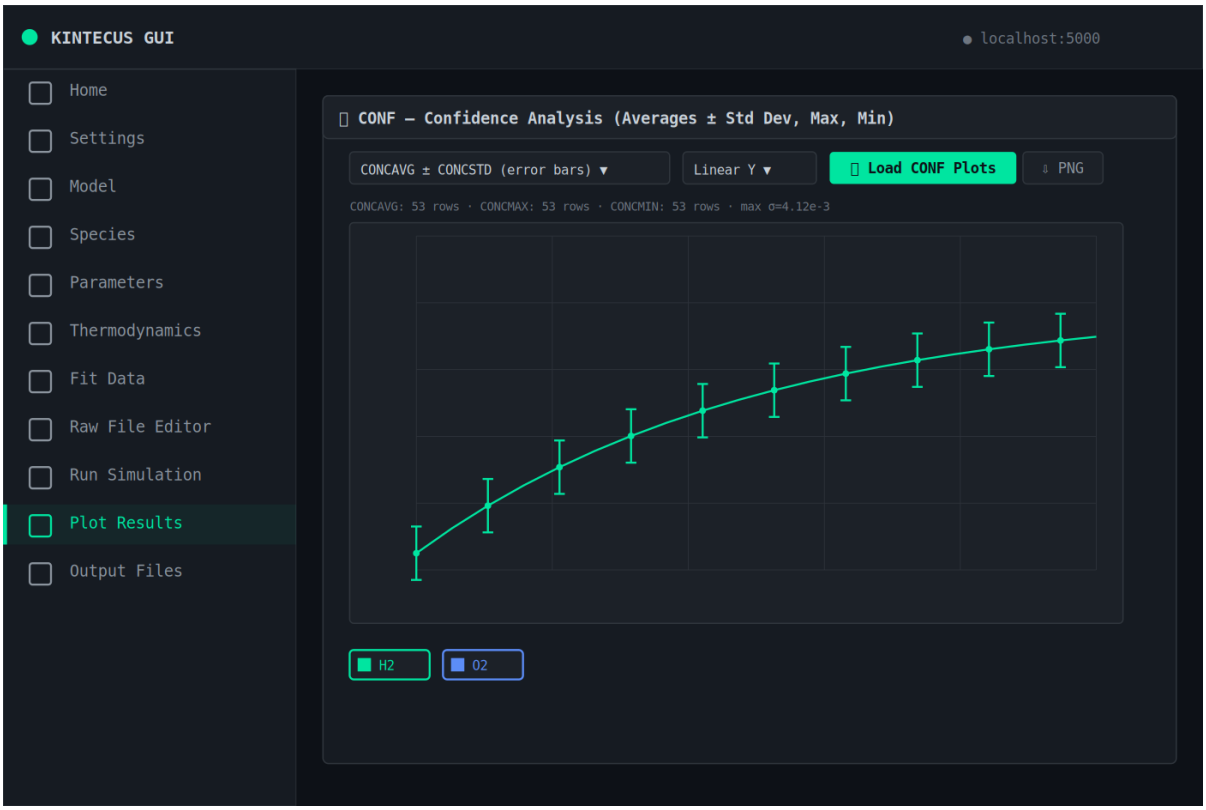

Figure 12. CONF panel — CONCAVG with CONCSTD plotted as symmetric vertical error bars.

- CONCAVG ± CONCSTD — mean concentrations with symmetric error bars (upper = avg + std, lower = avg − std).
- CONCMAX — maximum concentrations across the Monte-Carlo runs. No error bars.
- CONCMIN — minimum concentrations across the Monte-Carlo runs. No error bars.
- Linear / Log Y toggle and PNG export.
- Status line shows the global maximum σ for diagnostic purposes — if max σ = 0 your CONF data has no spread.
- If any of CONCAVG.TXT, CONCSTD.TXT, CONCMAX.TXT, or CONCMIN.TXT is missing the panel reports exactly which file is absent.

11e. Scan Plot (SCANPLOT)

Appears only when -scan is in the switches. A composite of every CONCnnnnnn.TXT file produced by a scan run. The file count is read from SCANS.TXT but the GUI also globs the directory to handle partial runs.

Figure 13. SCANPLOT — composite view of all parameter-scan runs on one chart.

- All scans appear on a single chart with the same time axis. Each species gets its own color shared across scans.
- Species toggles — clicking H2 hides every scan of H2 at once.
- Scan toggles (shown when there are 20 or fewer scans) — hide individual scan runs.
- Transparency is auto-adjusted based on scan count so overlapping lines remain distinguishable.

11f. Chemical Network Diagram

Appears only when -CHEMNET is in the switches and Kintecus actually produced chemnetwork.png or chemnetwork.jpg. The image is embedded directly on the page.

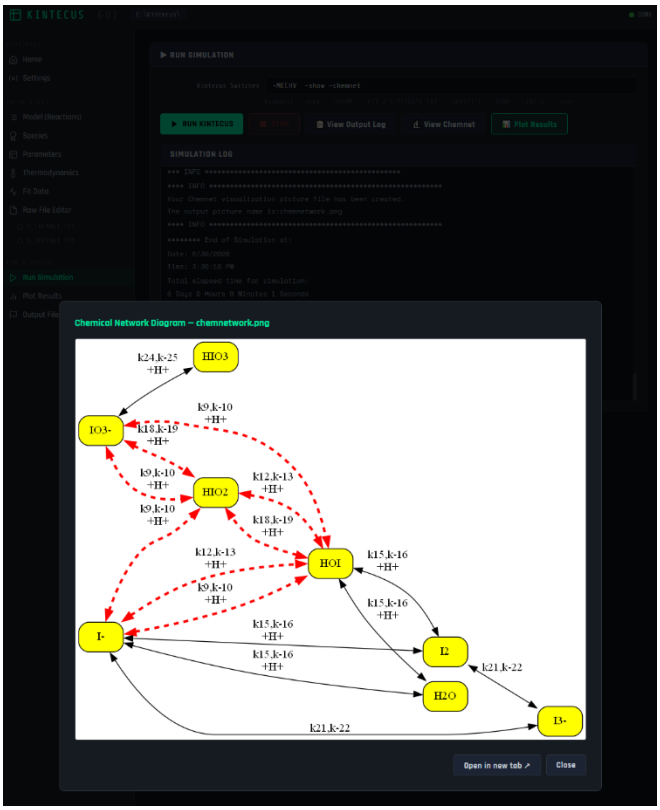

Figure 14. Chemical network diagram — Kintecus-generated graph of species and reaction pathways.

- The image also pops up automatically the moment a -CHEMNET run finishes.
- Click "Open in new tab ↗" to view the full-resolution image in a separate browser tab.

12. Kintecus Key & KINKEY.TXT

Some Kintecus features require a license key. The GUI has a dedicated Kintecus Key field on the Settings page (max 60 characters).

- If the field contains at least 10 characters when you click Run Kintecus, the GUI writes KINKEY.TXT to your Kintecus path before launching the binary. The file contents are the key string plus a trailing CRLF.
- If the field has fewer than 10 characters the file is not written, and Kintecus uses whatever KINKEY.TXT is already on disk (or none).
- The key is stored in your .kintpack files for portability.

13. Tips, Troubleshooting & Workflow

Recommended Workflow

1. Open the GUI and set Kintecus Path on the Settings page (one-time setup).
2. Build or load your Model grid. Use Make Species from Model to bootstrap Species if you're starting fresh.
3. Fill in Parameters, Thermodynamics, and Fit Data as needed.
4. Add any O_ files (e.g. FITDATA1.TXT, FITDATA2.TXT for multi-fit runs).
5. Save a kintpack so you have a clean restore point.
6. Adjust switches on the Run Simulation page and click ▶ RUN KINTECUS.
7. When the run completes, navigate to Plot Results — the relevant analysis panels appear automatically.
8. Your output files from a Kintecus run, such as concentrations (CONC.TXT), optimized/regressed values (OPTOUT.TXT), NSA files, or anything Kintecus creates are **NOT SAVED** with the Kintpack file. You have to manually copy or rename those!

Common Issues

"kintecus.exe not found"

Either the Kintecus Path in Settings is wrong, or the main Kintecus package was not installed before the GUI installer was run. Verify kintecus.exe lives in C:\Kintecus\ (or whatever path you specified).

Plot Results page is mostly blank

Switches like -FIT, -CONF, -SENSIT, -scan, and -CHEMNET each gate a separate plot panel. If you only ran a basic simulation, only the main concentration chart will appear — that is expected.

"Switches X, Y are mutually exclusive"

You have two of -SCAN, -SENSIT, -FIT, or -CONF on the same command line. Remove one. The GUI deliberately enforces this rule because Kintecus cannot produce coherent output when these modes are combined.

Large simulations freeze the browser

25+ MB of standard-output text will overwhelm any browser. The GUI caps the visible log at 500 lines (oldest are pruned) and only sends incremental updates over the network, but if you have an extremely chatty run consider removing the -show switch — the full output is still saved to view.txt regardless.

SENSIT heatmaps appear all-gray

Check the status line — if it reads "global ±1.84e+3" (or some huge number) you have a numerical outlier washing out the color scale. The GUI uses 99th-percentile clipping to mitigate this; if it still looks washed-out, examine your SENSITnnn.TXT files for instability.

Restart Tips

- If something looks stuck, close the browser tab and refresh — the GUI is stateless on the browser side; everything is in the .kintpack you saved.
- If the Python/Flask server itself misbehaves, close it (Ctrl+C in the console window or close the window) and relaunch kintecus_gui.exe.
- All your editable state lives in either the .kintpack file or in the DAT/TXT files in the Kintecus directory — nothing important lives in the running server process.

Where to Save Important Things

- Your project state → in a .kintpack file (download to your Documents folder, OneDrive, USB, etc.).
- Your Kintecus inputs → automatically written to the Kintecus directory before each run.
- Your Kintecus outputs → also live in the Kintecus directory. Use  Export All as JPEG (SENSIT) and ⇩ PNG buttons on the chart panels to capture publication-quality images.

14. Convert Kintecus-Excel to KintecusGUI

The entire Kintecus-Excel Worklbook can be stored in the Kintecus GUI. Start in the Kintecus-Excel Workbook, click “RUN” (assuming you have a Kintecus Unlocking Key) on the CONTROL worksheet and then press “CTRL-C” or “CTRL-BREAK” or close the scrolling text windows that pops up. When one clicks “RUN”, yhe VBA macros in the Kintecus-Excel workbook will automatically output the tab-delimited text files, MODEL.DAT, SPECIES.DAT, PARM.DAT, THERM.DAT, TRANSPORT.DAT, fitdata.txt and any worksheet that starts with “O_<name>” as also tab delimited text file(s) <name>.

Now one just has to manually load each of these files into the KintecusGUI. One can now go in the KintecusGUI and click on the “Model Page” and click the “LOAD MODEL.DAT” button and the entire model file will be loaded into the grid. Now go in the “Species Page” and click on the “LOAD SPECIES.DAT” button and the entire species file will be loaded. Do this for the “Parameters” page, Thermodynamics (if appropriate), Fitdata. The text files <name> that were outputted can each individually be loaded as described in the “O_ Perturbation / Fit-Data Files (bottom section)”. Don’t forget to copy the Kintecus command line options and comments into “Settings” page and the “Run Simulation” page ! One can now save the entire system as a “kintpack” file for easy loading, modifying and running.

— End of Guide —