

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Initializing...

Registered S3 method overwritten by 'sensitivity':
method from
print.src.dplyr

The screenshot shows the Thermosimfit application window. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains three input fields: 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_a(HD) [1/M]' (3000000). An 'Advanced options' button is shown below these. The 'Boundaries' section contains six input pairs for concentration boundaries: K_a(HG) (lower: 10, upper: 1e+08), I(0) (lower: 0, upper: 1e+08), I(HD) (lower: 0, upper: 1e+08), and I(D) (lower: 0, upper: 1e+08). Below these sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. A large 'Sensitivity analysis' dialog box is open at the bottom, containing a ' +/- boundary in [%]' input field (set to 15), a 'Start Sensitivity analysis' button, a 'Cancel' button, a 'Save result of sensitivity analysis' button, and a status message 'Initializing...'. A pink status bar at the bottom right displays the message 'Registered S3 method overwritten by 'sensitivity': method from print.src.dplyr'.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 1%

Registered S3 method overwritten by 'sensitivity':
method from
print_src.dplyr

This screenshot shows the Thermosimfit software interface. The left sidebar contains model selection and information buttons. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). An 'Advanced options' button is present. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A 'Sensitivity analysis' dialog is open, showing '+/- boundary in [%]' set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. It also displays 'Completed: 1%'. A status message at the bottom right indicates a registered S3 method 'print_src.dplyr' has been overwritten by 'sensitivity'.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 3%

Registered S3 method overwritten by 'sensitivity':
method from
print_src dplyr

The screenshot shows the Thermosimfit application window. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main area has two tabs: 'Parameter' and 'Boundaries'. Under 'Parameter', there are three input fields: 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_a(HD) [1/M]' (3000000). An 'Advanced options' section is partially visible. Under 'Boundaries', there are six input fields for concentration boundaries: K_a(HG) lower (10), K_a(HG) upper (1e+08), I(0) lower (0), I(0) upper (1e+08), I(HD) lower (0), and I(HD) upper (1e+08). Below these tabs are buttons for Optimization, Sensitivity analysis (which is active), and Batch processing. A 'Sensitivity analysis' dialog is open, showing '+/- boundary in [%]' set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. It also displays 'Completed: 3%'. A status message at the bottom right indicates a registered S3 method for 'sensitivity'.

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 4%

Registered S3 method overwritten by 'sensitivity':
method from
print_src dplyr

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 5%

Registered S3 method overwritten by 'sensitivity':
method from
print_src_dplyr

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model

Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 7%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two main sections: Parameter and Boundaries.

Parameter Section: Contains fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). An "Advanced options" button is present.

Boundaries Section: Contains boundary settings for K_a(HG), I(0), I(HD), and I(D) values, both for lower and upper bounds.

Sensitivity Analysis Section: Shows a "+/- boundary in [%]" input field set to 15, and buttons for "Start Sensitivity analysis", "Cancel", and "Save result of sensitivity analysis". It also displays a progress bar indicating "Completed: 7%".

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model
Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and Info. The main area is divided into two sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an Advanced options button. The Boundaries section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis section shows a progress bar at 0% completion and a large empty rectangular area for results.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%



Thermosimfit

☰

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model

Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 11%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a menu icon. On the left, a sidebar lists models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' section with a plus sign. The 'Boundaries' section contains ranges for K_a(HG), I(0), I(HD), and I(D) values. At the bottom, tabs for Optimization, Sensitivity analysis (which is active), and Batch processing are shown. The 'Sensitivity analysis' section includes a '+/- boundary in [%]' input (15), 'Start Sensitivity analysis' and 'Cancel' buttons, and a progress bar indicating 'Completed: 11%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 13%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar indicates the completion of a sensitivity analysis at 13%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 14%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task has completed 14%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 15%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 17%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 18%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 20%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is completed at 20%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HG)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M]
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 21%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 23%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 24%



Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model

Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 26%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a sidebar with model selection (Data import, DBA models, GDA model, IDA model) and an 'Info' button. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' section contains ranges for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a progress bar at 26% completion and a note about +/- boundary in [%] (15%). Buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis' are present.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 27%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 27%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 29%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 30%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a menu icon. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains three input fields: 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_a(HD) [1/M]' (3000000). It also features an 'Advanced options' button. The 'Boundaries' section contains six input fields for concentration boundaries: K_a(HG) lower (10), K_a(HG) upper (1e+08), I(0) lower (0), I(0) upper (1e+08), I(HD) lower (0), and I(HD) upper (1e+08). Below these sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. The 'Sensitivity analysis' section includes a '+/- boundary in [%]' input (15), a 'Start Sensitivity analysis' button, a 'Cancel' button, a 'Save result of sensitivity analysis' button, and a progress bar indicating 'Completed: 30%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 32%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' section with a plus sign. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' tab shows a progress bar at 32% completion. At the bottom, there are buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 33%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' section with a plus sign. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 33%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 35%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 36%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 38%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M]
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 40%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 41%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 41%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 42%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 44%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 44%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 45%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar at the bottom indicates the Sensitivity analysis is completed at 45%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 47%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar at the bottom indicates the sensitivity analysis is 47% completed.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M]
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 49%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and $K_s(HD)$ [1/M] (3000000). It also has an 'Advanced options' section. The 'Boundaries' section allows setting boundaries for $K_s(HG)$, $I(0)$, $I(HD)$, and $I(D)$. Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange box highlights the 'Sensitivity analysis' section, which shows a progress bar at 49% completion. The progress bar area contains a large empty orange rectangle.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 50%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 52%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 53%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 53%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 55%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 55%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 56%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' section with a plus sign. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is 56% completed.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 58%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 59%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that the 'Sensitivity analysis' task is 59% completed.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 61%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 63%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 64%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' section with a plus sign. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates the Sensitivity analysis is completed at 64%. The bottom right corner features a large orange rounded rectangle.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 66%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar at the bottom indicates the Sensitivity analysis is 66% completed.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 67%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar at the bottom indicates the sensitivity analysis is 67% completed.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 69%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 70%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 70%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 72%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M], Dye conc. [M], and K_a(HD) [1/M]. The 'Boundaries' section allows setting lower and upper bounds for K_a(HG), I(0), I(HD), and I(D). Below these are tabs for Optimization, Sensitivity analysis (which is currently active), and Batch processing. A large orange progress bar indicates the completion of a sensitivity analysis at 72%.

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model

Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 74%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two main sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an Advanced options button. The Boundaries section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis section shows a progress bar at 74% completion and a note about +/- boundary in [%] (15%). It also has Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis buttons.

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model

Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 75%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two main sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an Advanced options button. The Boundaries section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis tab shows a progress bar at 75% completion. It includes a +/- boundary in [%] input field (15), Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis buttons.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 77%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M], Dye conc. [M], and K_a(HD) [1/M]. The 'Boundaries' section includes fields for K_a(HG), I(0), I(HD), and I(D) values, both with lower and upper boundaries. Below these sections is a navigation bar with tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 77%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 79%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for different models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange box highlights the 'Sensitivity analysis' tab and its associated parameters.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The top navigation bar includes 'Thermosimfit' and a menu icon. On the left, a sidebar lists various models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below this is an 'Info' button. The main workspace is divided into two main sections: 'Parameter' and 'Boundaries'. The 'Parameter' section contains three input fields: 'Host conc. [M]' (0.000001), 'Dye conc. [M]' (0.000001), and 'K_a(HD) [1/M]' (3000000). It also features an 'Advanced options' button. The 'Boundaries' section contains six input fields for concentration boundaries: K_a(HG) and I(0) both have lower bounds of 0 and upper bounds of 1e+08; I(HD) has a lower bound of 0 and an upper bound of 1e+08; and I(D) has a lower bound of 0 and an upper bound of 1e+08. Below these sections are tabs for 'Optimization', 'Sensitivity analysis' (which is currently selected), and 'Batch processing'. The 'Sensitivity analysis' section includes a '+/- boundary in [%]' input field set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 0%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

Thermosimfit

Data import
DBA (const. host) model
DBA (const. dye) model
GDA model
IDA model

Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options

Boundaries

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two main sections: Parameter and Boundaries. The Parameter section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000), with an Advanced options button. The Boundaries section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis section shows a '+/- boundary in [%]' input field set to 15, and buttons for Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis. It also displays a progress bar indicating 'Completed: 0%'.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_s(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_s(HG)$ value lower boundary [1/M]
10

$K_s(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains model selection and information buttons. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and $K_d(HD)$ [1/M] (3000000). An 'Advanced options' button is present. The 'Boundaries' section includes fields for $K_d(HG)$ boundaries (lower: 10, upper: 1e+08) and $I(0)$ and $I(D)$ boundaries (lower: 0, upper: 1e+08). Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar indicates the completion of a sensitivity analysis at 0%.

Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries (both 10 and 1e+08), I(HD) lower and upper boundaries (both 0 and 1e+08), and I(D) lower and upper boundaries (both 0 and 1e+08). Below these sections are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A large orange progress bar at the bottom indicates the completion of a sensitivity analysis task at 0%.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M] ⓘ Help
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 0%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel ⚙ Save result of sensitivity analysis

Completed: 99%

This screenshot shows the Thermosimfit software interface. The left sidebar contains navigation links for various models and an info button. The main area is divided into two sections: 'Parameter' and 'Boundaries'. The 'Parameter' section includes fields for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000). It also has an 'Advanced options' button. The 'Boundaries' section allows setting boundaries for K_a(HG), I(0), I(HD), and I(D) values. Below these are tabs for Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange box highlights the 'Sensitivity analysis' section, which shows a progress bar at 99% completion. It includes fields for +/- boundary in [%] (15), buttons for Start Sensitivity analysis and Save result of sensitivity analysis, and a status message.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 92%



Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 94%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 95%

This screenshot shows the Thermosimfit software interface. The left sidebar contains model selection and info buttons. The main area has two tabs: 'Parameter' and 'Boundaries'. In 'Parameter', values for Host conc. [M] (0.000001), Dye conc. [M] (0.000001), and K_a(HD) [1/M] (3000000) are set. An 'Advanced options' section is partially visible. The 'Boundaries' tab shows ranges for K_a(HG), I(0), I(HD), and I(D). Below these tabs is a navigation bar with Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange box highlights the 'Sensitivity analysis' section, which displays a progress bar at 95% completion. The bottom of this section includes buttons for Start Sensitivity analysis, Cancel, and Save result of sensitivity analysis.

Thermosimfit

☰

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

$K_{d}(HD)$ [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

$K_d(HG)$ value lower boundary [1/M]
10

$K_d(HG)$ value upper boundary [1/M]
1e+08

$I(0)$ value lower boundary
0

$I(0)$ value upper boundary
1e+08

$I(HD)$ value lower boundary [1/M] ⓘ Help
0

$I(HD)$ value upper boundary [1/M]
1e+08

$I(D)$ value lower boundary [1/M]
0

$I(D)$ value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 97%



Thermosimfit

☰

■ Data import
■ DBA (const. host) model
■ DBA (const. dye) model
■ GDA model
■ IDA model

ⓘ Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

Advanced options +

Boundaries ⓘ Help

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

Optimization Sensitivity analysis Batch processing

Sensitivity analysis

+/- boundary in [%]
15

Start Sensitivity analysis Cancel Save result of sensitivity analysis

Completed: 99%

This screenshot shows the Thermosimfit software interface. The left sidebar contains model selection and info buttons. The main area has two tabs: 'Parameter' and 'Boundaries'. In 'Parameter', three values are set: Host conc. [M] at 0.000001, Dye conc. [M] at 0.000001, and K_a(HD) [1/M] at 3000000. An 'Advanced options' section is collapsed. In 'Boundaries', ranges for K_a(HG), I(0), I(HD), and I(D) are defined. Below these tabs is a 'Sensitivity analysis' section with a '+/- boundary in [%]' input set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is completed at 99%. A large orange-outlined rectangular box covers the bottom half of the central workspace.

Thermosimfit

- Data import
- DBA (const. host) model
- DBA (const. dye) model
- GDA model
- IDB model
- Info

Parameter

Host conc. [M]
0.000001

Dye conc. [M]
0.000001

K_a(HD) [1/M]
3000000

[Advanced options](#)

Boundaries

K_a(HG) value lower boundary [1/M]
10

K_a(HG) value upper boundary [1/M]
1e+08

I(0) value lower boundary
0

I(0) value upper boundary
1e+08

I(HD) value lower boundary [1/M]
0

I(HD) value upper boundary [1/M]
1e+08

I(D) value lower boundary [1/M]
0

I(D) value upper boundary [1/M]
1e+08

[Optimization](#)
[Sensitivity analysis](#)
[Batch processing](#)

Sensitivity analysis

+/- boundary in [%]
15

[Start Sensitivity analysis](#) [Cancel](#) [Save result of sensitivity analysis](#)

Completed: 99%

Parameter	Estimated fraction of solute	Error (approx.)
K _a (HG)	~0.10	±0.15
I ₀	~0.10	±0.15
HD ⁺	~0.25	±0.15
D ⁻	~0.25	±0.15
K _a (HD) ⁺	~0.25	±0.15
K _a (D) ⁺	~0.10	±0.15
I(D)	~0.10	±0.15
HD ⁰	~0.10	±0.15