

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 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 is an 'I(D)' section with similar boundary inputs. At the bottom, there are tabs for 'Optimization', 'Sensitivity analysis' (which is currently 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'. A status message 'Initializing...' is displayed. A pink tooltip on the right provides information about registered methods. The overall interface is clean with orange and grey accents.

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ⓘ 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 for 'sensitivity'.

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■ Data import
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ⓘ 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 currently 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]
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%

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: 0%'. A status message at the bottom right indicates a registered S3 method for 'sensitivity'.

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■ 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 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 10 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 (set to 15), a 'Start Sensitivity analysis' button, a 'Cancel' button, a 'Save result of sensitivity analysis' button, and a progress bar indicating 'Completed: 7%'. A large orange-outlined rectangular area is present in the bottom right corner of the main workspace.

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

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: 10%

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. A progress bar indicates the task is completed at 10%.

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 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: 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: 12%

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 panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel 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' panel 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 panels are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows a progress bar at 12% 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: 14%

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, having completed 14%.

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: 15%

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. 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'. A progress bar indicates the task is completed at 15%. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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

Completed: 1%

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: 21%

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) and I(0) values (lower and upper bounds both at 10 and 1e+08), I(HD) values (both at 0 and 1e+08), and I(D) values (both at 0 and 1e+08).

At the bottom, there are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The Sensitivity analysis section includes a "+/- boundary in [%]" input (set to 15), a "Start Sensitivity analysis" button, a "Cancel" button, a "Save result of sensitivity analysis" button, and a status message "Completed: 21%".

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: 22%

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. 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'. A progress bar indicates the task is 'Completed: 22%'. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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

$K_s(HD)$ [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: 25%



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 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. A progress bar indicates the task is completed at 26%. A large orange-outlined rectangular area is overlaid on the bottom half of the screen.

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: 28%



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

☰

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: 30%



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: 34%

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 34%.

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: 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

☰

■ 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: 38%

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 38% 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: 39%



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

☰

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: 43%



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 Data import, DBA models, GDA model, IDA model, and an Info section. The main area is divided into two panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel 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' panel 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 panels 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 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: 46%

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 active), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 46%.

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: 48%

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 48%.

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: 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_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 49%.

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: 51%

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 active), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 51%.

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

☰

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: 54%



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 different models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below these are links for Info and Advanced options. 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). Below these is a 'Advanced options' button. The 'Boundaries' section contains six input fields for chemical equilibrium constants and initial concentrations. At the bottom, there are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A progress bar indicates that the Sensitivity analysis has completed 56%.

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: 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

$K_{d}(HD)$ [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: 60%

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 $K_{d}(HD)$ [1/M] (3000000). It also has an 'Advanced options' section. The 'Boundaries' section allows setting boundaries for $K_{d}(HG)$, $I(0)$, $I(HD)$, 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 60% completion. It includes fields for +/- boundary in [%] (15), buttons for Start Sensitivity analysis and Save result of sensitivity analysis, and a message indicating the task is 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: 61%

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 active), and Batch processing. A large orange progress bar at the bottom indicates that a sensitivity analysis is in progress, completed at 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

☰

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: 64%



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). 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 66%.

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 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 67%.

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 different models: Data import, DBA (const. host) model, DBA (const. dye) model, GDA model, and IDA model. Below these are links for Info and Advanced options. 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 includes an 'Advanced options' button. The Boundaries section contains fields for K_a(HG) and I(0) boundaries (both lower and upper bounds set to 10 and 1e+08 respectively), I(HD) and I(D) boundaries (both lower and upper bounds set to 0 and 1e+08 respectively). 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 70%.

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: 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 ⓘ 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: 73%

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 panels: 'Parameter' and 'Boundaries'. The 'Parameter' panel 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' panel includes fields for K_a(HG) and I(0) lower and upper bounds (both 10 and 1e+08), I(HD) lower and upper bounds (both 0 and 1e+08), and I(D) lower and upper bounds (both 0 and 1e+08). Below these panels are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. The 'Sensitivity analysis' section shows '+/- boundary in [%]' set to 15, and buttons for 'Start Sensitivity analysis', 'Cancel', and 'Save result of sensitivity analysis'. A progress bar indicates the task is 'Completed: 73%'. A large orange-outlined rectangular placeholder is present in the bottom right corner.

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: 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.

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.

At the bottom, there are tabs for Optimization, Sensitivity analysis (which is currently selected), and Batch processing. A progress bar indicates the Sensitivity analysis is completed at 75%.

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: 76%



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: 78%

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 78%.

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. 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'. A progress bar indicates the task is 'Completed: 0%'. A large orange-outlined rectangular box 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: 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) 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: 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

☰

■ 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

☰

■ 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 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 collapsed. In 'Boundaries', ranges for K_a(HG), I(0), I(HD), and I(D) are defined. Below these tabs is a navigation bar with Optimization, Sensitivity analysis (which is active), and Batch processing. A large orange progress bar at the bottom indicates the 'Sensitivity analysis' is completed at 0%. The bottom right corner features a large orange rounded rectangle.

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: 0%



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: 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 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. The 'Sensitivity analysis' tab shows a progress bar at 99% completion. It also has 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: 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

$I(HD)$ 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: 99%



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: 95%



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: 96%

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 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. The Sensitivity analysis panel shows a progress bar at 96% 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: 99%

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). The 'Boundaries' section includes fields for K_a(HG) and I(0) lower and upper boundaries, and I(HD) and I(D) lower and upper boundaries, all set to 10 or 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 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: 99%

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 active), and Batch processing. A large orange progress bar at the bottom indicates the Sensitivity analysis is completed at 99%.