SAM SAGE Igor Tool

SAM SAGE - Software for Analysis of GCMS and EGA - was developed to aid in the analysis of SAM flight model data. SAGE will be used to model undersampled GCMS and complicated EGA data, calculate mass spectra based on modeled GCMS data, and determine peak onset temperature, peak maximum temperature, and peak area of modeled EGA data.

Latest

Use the #igorpro channel of the SAM-MSL Slack for help requests and discussion.

Igor 8 requires SAGE 1.8.4 or higher.

Software: SAGE1.8.4.pxp

Documentation/History

Manual: SAGEManualv1.3.pdf

SAGE new features.pptx in 1.7

Selected new features in 1.2, presented at the GCMS focus group meeting: SAGE_update_09_20_12.pptx

SAGE Release History

Data Preparation

The data that SAGE requires can be checked out from XINA and takes the form of a file named IGORdata.zip. Use 'Checkout All' or 'Checkout Secondary' to retrieve it. Unzip the archive inside the TID folder, and then load the TID folder from SAGE using the "Macros/Load TID Folder" menu item.

All SAM runs with QMS data should have an IGORdata.zip file generated and available alongside the tm.sam file. If there is one missing let the PDL team know.

Quickstart

1. If you don't have IGOR Pro, install it from Wavemetrics
2. Double-click the .pxp file of the latest version of SAGE

3. Save the .pxp file with a new name
4. Under the Macro menu select "Load TID Folder" and navigate to the TID folder you want to look at
5. Try out SAGE's data processing capabilities
    - Check the TM Msgs to determine which EM was used, in order to select the correct coefficients for deadtime correction (v1.2 only)
    - Optionally display TM markers and other overlay data
    - Drag the vertical lines to set a background region
    - Display different data corrections with the dropdown menu at the top left
    - Use the Plot tab to add/remove bands and masses from the graph
    - Select peak regions in the Peak tab
    - Open Peak Graph window with the Magnify button
        - In Time tab, adjust time range of peak region, if necessary
        - In Mass tab, select set of masses and bands to use in fit
        - In Fit tab, select fit function, choose initial peak parameters, and click Fit
        - Display mass spectra of fitted peaks, with options to output to NIST 11 format text file
        - In Review tab (> tab, v1.2 only), quickly compare the "raw" data to the fitted data of a single mass (or a single band) at a time
    - Export all fitted peaks to a chromatogram (in a .jdx format text file, which is compatible with ACD), with gaps between fitted peaks modeled with either a line fit or a moving average or connect data points.
6. Send any feedback to Micah Johnson and Anna Brunner

IGOR Tips

- Graph Interface
    - Click and drag marquee on plot, click inside marquee for Expand/Shrink options
    - Hover cursor over axis, scroll wheel to zoom in an out (side scroll slides data)
    - Option-Click to slide data with inertia, click to stop if it's still moving
    - Command-I shows cursors (drag cursors onto a wave in the graph to see info about the data point)
    - Command-T shows graph tools such as line or shape drawing capabilities
- KBColorizer Interface
    - If you close the 'Make Traces Different' window, newly added traces will be black.
    - Bring up the window again by selecting the last menu item in the Graph menu.
    - Nudging any of the three scroll bars in the Color Wheel section of that window will differentiate trace colors.
- Global Fit
    - If the fit does not converge, adjust the cursors if they seem off, or vary the value of the EMG modification factor. The following Igor-generated error messages are common and do not necessarily mean there is anything wrong with the data set or the program - they usually just mean the initial guesses weren't quite right. If you see these errors do not panic, just tweak the parameters. If they continue to occur, however, there may be something wrong besides the parameters.
        - "While executing FuncFit the following error occurred: singular matrix or other numeric error"
        - "While executing FuncFit the following error occurred: The fitting function returned NaN for at least one X value."
    - Global Fit does not do well if the peak you are trying to fit is not lined up precisely amongst the masses/bands - if there are slight time shifts, the fits do not look as good

Release History

Preview 1

- Import QMS count rates and marker data into waves
- Perform simple dead time correction
- Plot band data
- Selection of time range for background calculation

Preview 2

- Band and mass selection interface in Plot tab
  - Add/remove masses or bands by checking/unchecking the boxes
  - Highlighting a band automatically scrolls to corresponding mass range
  - Press up/down buttons to scroll quickly through masses and bands
  - Press spacebar when a mass or band is highlighted to quickly add or remove it

Preview 3

- In the Plot tab:
  - Quickly navigate between selected bands/masses by pressing j and k
  - In the mass list, masses corresponding to the highlighted band are color coded
- Peak selection interface in Peak tab:
  - Press "New" to select the time range of a peak using cursors
  - Rename peaks in peak list
  - Check box next to a peak name to highlight that range on the graph
  - Press "Magnify" to make a new Peak Graph window with a zoomed-in plot of the selected time range
- Peak Graph window:
  - In the Time tab, adjust time range of peak with cursors or text fields
  - In the Mass tab:
    - Set the sigma multiplier to specify a detection level (standard deviations above background)
    - Select/deselect masses and bands until the graph contains only the data with peaks at that time
  - In the Fit tab:
    - Select the peak center with the green square cursor, and the boundaries of the full-width half-maximum with the purple circle cursors
    - Press Reset to get cursors back if one gets accidentally dragged off the plot
    - Enter a modification (skew) factor if fitting to an Exponentially Modified Gaussian
    - Press Calc. Coeffs to generate guesses for the fit coefficients
    - Use calculated coefficients to perform a Global Fit

Version 1.0

- New peak fit functions: Lorentzian, exponentially-modified Gaussian
- Interface for entering initial guesses for multi-peak fit functions
- Simplified interface for calling Global Fit
- Method for quickly culling mass data that can't be fit
- Interpolation of GCMS data using fit coefficients
- Export file in JCAMP DX format, compatible with ACDLabs software
- Quick mass spectrum plot from fitted peak

Version 1.1

- Added peak fit check tab for looking at individual fit compared to mass data

Version 1.2

- Dead time correction interface and support for EM1/2 and custom coeffs
- Selective plotting of telemetry markers
- Implemented export tab
  - Set time range of export with cursor or time field
  - Snap cursor to visible marker
  - Fill-in data with line-fit or averaging option
  - Re-add background back to exported data
  - Show offset time as top axis of plot
- Remove bad fits from peak fit check tab
- Add prefix name to fit output waves so multiple fits can be saved

Version 1.3

- Support for IGORdata.zip archive
- Simple pyrolysis ramp temperature plotting from pyro_temp.log file
- EMG peak improvements
- Added "connect-the-dots" export capability for data that is not fit
- Command window readout for multiplier usage to assist with dead-time configuration
- Log/Linear plot toggle checkbox

Version 1.4

- Added 'Show Overlays' feature
  - Pyrolysis oven and sample temp plotting
  - GC temperatures and TCD signal plotting
- Plot mass vs temperature for EGA analysis from Pyro overlay tab

Version 1.5

- New overlays added
  - Low speed mux (HK1-154) data
  - Heater temperatures
  - MOT housekeeping data
  - Valve operations
- Support for dt.prms file
- Peak area calculations
- Support of band table update (1.5.2)

Version 1.6.1

- TLS housekeeping data overlay added

Version 1.7

- New macros: Smooth Data and Compare TIDs
- Additional option for custom_pyro_temp.txt file to define sample temperature

Version 1.8.1

- Igor 7 compatibility
- Pyro polyfit equations updated for TB and FM

Version 1.8.3

- Support for special files in TID
  - dt.prms - Dead time parameters
  - band_template.txt - Define masses that are contained in bands
  - fracmass.txt - Define special fractional masses that should appear in list checkbox interface
  - maptounit.txt - Defined fractional masses that should be mapped to unit masses

Version 1.8.4

- Igor 8 compatibility

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