

CARS Data Analysis Procedure

Dr. Luca M. L. Cantu

Luca.Cantu@dlr.de
+49 (0) 711 / 6862 257

DLR Stuttgart
Institute of Combustion Technology
Combustion Diagnostics Department

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1. Preparation

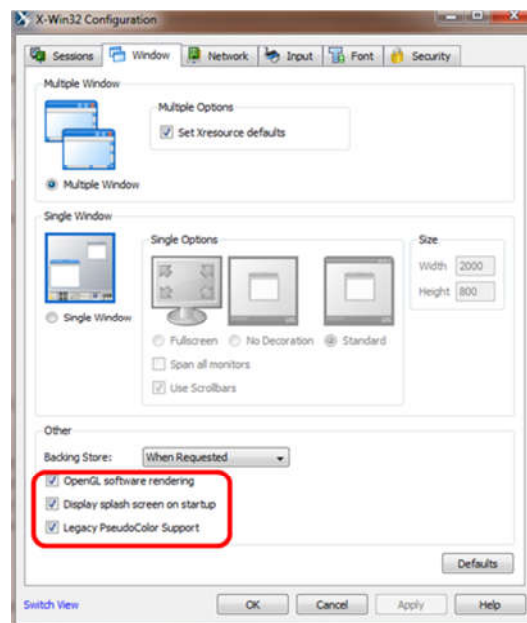
- Login to MC (AIX) machine via MC terminal using the following credentials:
 - Login: **vtmess**
 - Password: ask to SV-CARS system supervisor
 - Run **tcars03.e** (or the number of the MC terminal) to tell MC machine which terminal is connecting to it

To transfer the data from (or to) a Windows machine, use a file transfer protocol (FTP) software (**FileZilla** at DLR) and use as host address:

- **mc.vt.st.dlr.de**

Login and password are the same listed above.

It is also possible to connect remotely to MC machine through Windows systems; use **X-Win32** software and **telnet** connection type. Just remember to flag all the options in the window tab



- Create a directory on MC machine where to store all the raw data coming from DaVis software macro **Messung_svcars**. Note that the convention in use to name the data files is the following:

s8a086 is a sample of raw file, where:

- **s** = shifted
- **8** = last digit of the last year (e.g. 2008 = 8, 2016 = 6)
- **a** = average or e = einen pulse (single shot)

- 086 = day of the the year (varies from 001 to 365)
- Transfer the CARS data from DaVis computer to the MC terminal. A DaVis macro, **filecopy("E:\\hdc_brenner\\"+svcars_daydir);**, was created to avoid manual transfer. In any case, for each measurement point the following files must be present inside the designated folder in MC machine:
 - **.asc** = raw ASCII data
 - **.log** = header information (e.g. laser energies, location of measurement, etc...)
 - **.tst** = measurement protocol
- To make the scroll bar appears, type the following command:
 - **xterm -sb -sl 500 &**
- Run program setdir.e to copy from an old directory all the required codes and respective folders.
 - **setdir.e [old directory] [new directory]**

The following folders will be copied with the respective codes (no data):

- **apfit** folder designated to create/modify the slit (instrument) function
 - **carp** folder designated to create/modify the dispersion (wavenumber/pixel)
 - **lfit** folder designated for the fitted data (results): use inputs from quick fit and library fit
 - **lflib** folder designated to library creation and library fit
 - **mess** folder designated to correct the raw data for dye curve and background subtraction
 - **qflib** folder designated to quick fit to select the best methods for fitting
- Useful commands for MC terminal:
 - **dir** lists all the files/folders inside the directory (same as Windows)
 - **cat** opens and print a file on screen
 - **pq** opens and print a file on screen but stops at the end of each page
 - **up** moves one directory up (or use the command **cd..** as in Windows)
 - **ho** moves back to the designated home directory
 - **mv** rename a file
 - **dfu** shows the size of folders
 - **xterm &** opens a new terminal leaving active the old one (they can be used simultaneously)
 - **pwd** shows the actual directory
 - **ne** opens the file editor
 - **mkdir** makes a new folder (same as Windows)
 - **cp -p** copies as original in a new folder
 - **ls *** shows only file with designate extension (e.g. **ls *.e** show only **.e** files)
 - **gm** shortcut to **mess** folder
 - **ga** shortcut to **apfit** folder
 - **gqf** shortcut to **qflib** folder
 - **gl** shortcut to **lfit** folder
 - **glf** shortcut to **lflib** folder
 - **gc** shortcut to **carp** folder
 - **chmod u+x *.e** gives the right to use all the executables inside the working folder
 - **asctommf [input.asc] [output.mmf]** converts input files in **.asc** to a **.mmf** file

2. Correction for dye curve and background

- Work inside **mess** folder
- Edit **ne set.e** (code which creates input files for all other programs) code:
 - **TAG** = day of the year (as in the name of raw data)
 - **DATUM** = date
 - **DIRNAM** = name of the directory
 - **export LIN_SLO** = non-linearity slope of the detector (modify only if unsatisfactory fit)
 - **export LIN_OFF** = non-linearity offset of the detector (modify only if unsatisfactory fit)

```

# set.e 19-Feb-98
-----
export TAG=137
export DATUM=17-May-13
export DIRNAME="/data2/cv/vt/mess/mess/spray"
export PRE=s3
export PRE1=s3
export DIRMESS=${DIRNAME}/${PRE}a${TAG}/mess/
export DIREXP=${DIRNAME}/${PRE}a${TAG}/
export DIRAPFIT=${DIRNAME}/${PRE}a${TAG}/apfit/
export DIRQFLIB=${DIRNAME}/${PRE}a${TAG}/qflib/
export DIRFLIB=${DIRNAME}/${PRE}a${TAG}/flib/
export DIRLFIT=${DIRNAME}/${PRE}a${TAG}/lfit/
export DIRCARP=${DIRNAME}/${PRE}a${TAG}/carp/
export DIRSD=${DIRNAME}/${PRE}a${TAG}/mess/
# for 1 pixel/group:
# export LIN_SLO=.0900261
# export LIN_OFF=.632366
# for 2 pixel/group:
export LIN_SLO=.096368
export LIN_OFF=.58588

```

After setting all the required parameters according to the new dataset, run the code.

- **set.e**
- Modify **set-nr.e** and set a range where N_2 is located in order to maintain the peak of the intensity as it was during the experiment:
 - **SDEVSTART** = minimum number of pixel where to find N_2 peak
 - **SDEVEND** = maximum number of pixel where to find N_2 peak
- Run **korsp-nr.e** (code to correct single shots for dye curve and background subtraction) code:
 - **korsp-nr.e [run # where the dye curve was saved] [# of dye curve to be saved]**
e.g. korsp-nr.e 02 01

This code creates the following outputs:

- **xxmyyy.asc** corrected and normalized dye curve (ASCII)
- **xxnyyy.asc** normalized, relative single dye curves (ASCII)
- **xxuyyy.asc** background for dye curve (ASCII)
- **tnyyy.asc** normalized, relative single dye curves (ASCII)
- **dyexx.asc** corrected averaged dye curve (ASCII), only for visualization

To see and decide which dye curve use for the data analysis, run the **spi** code.

Here some useful commands for spi:

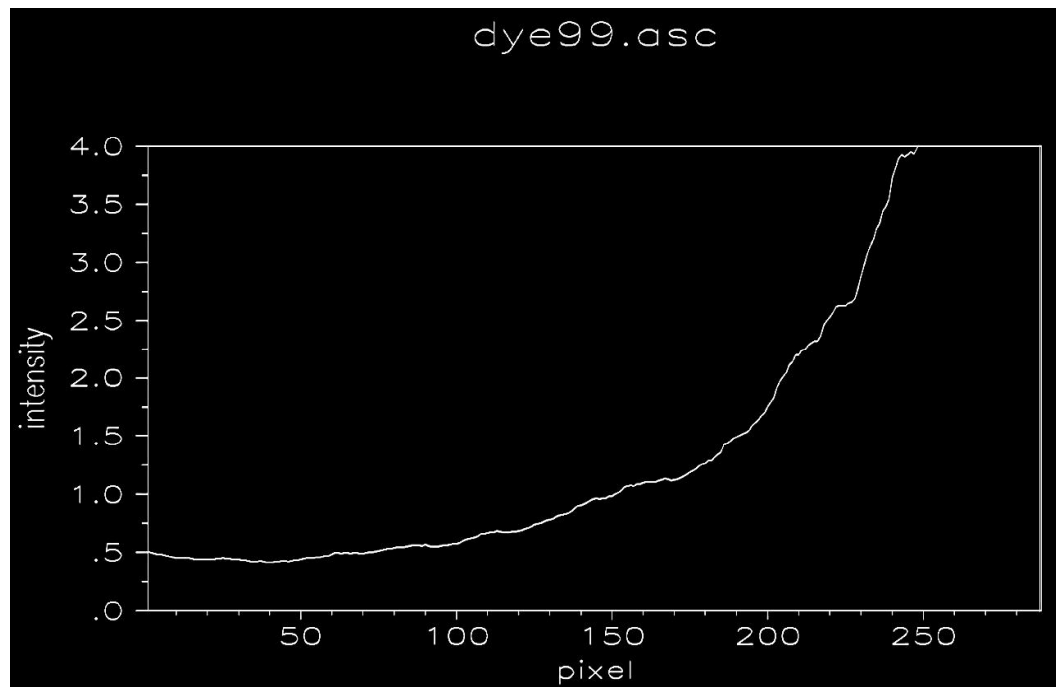
- **chd [file]** changes the default work file (e.g. chd s9m31101.asc)
- **gino** displays data (e.g. gin-(parameter1)-(parameter2), gin-asc-yma4)
- **load [file]** loads a file and keep into memory
- **load [file]-mean** loads a file and average with the one(s) in memory
- **unlock** unlocks all the file and enable modifications
- **sd** adds description to the head of the plot
- **save [filename]** saves the file in use with the chose filename (and extension)
- **gin-asc** displays ASCII format
- **gin-mmfm** displays mmf (binary) format
- **gin-ymaX** sets y-maximum (X = maximum value, usually between 2 and 4)
- **gin-yminX** sets y-minimum (X = minimum value, usually -500)
- **gin-xmaX** sets x-maximum (X = maximum value, usually between 2 and 4)
- **gin-xminX** sets x-minimum (X = minimum value, usually -500)
- **gin-lasX** plots last files in one single graph (X = number of plots)
- **gin-pform pq** generates the postscript
- **@spek** displays all spectra in separated boxes
- **@fit** displays all the data, fitted spectra and difference in separated boxes
- **gin-mul** displays multi spectra (e.g. gin-mmfm-mul-las20)
- **nomul** disables multiple plots (just a single plot with -eventually- multiple lines)
- **gin-ps** saves a copy of the plots in **.ps** format
- **charli X z2su** prints spectrum (X = filename)

e.g. To visualize the summary of dye curves use the following command sequences:

1. spi
2. chd dyexx.asc
3. gin-asc-yma4-fir1-las4 (open first 4 plots in gino ASCII format with ymax=4)

Note the color scale sequence:

- 1st curve is white
- 2nd curve is red
- 3rd curve is blue



Run this code for all the dye curves recorded during the experiment. Verify that there is no significant changes between the begin and the end of the experiment; if so, additional correction need to be performed based on interpolation of the dye curve change during the experimental time.

e.g. To average to dye curves, use the following command sequences:

1. spi
2. chd dyexx.asc
3. unlock
4. load dyexx.asc (loads first dye curve)
5. load dyexx.asc-mean (loads second dye curve and average with the first one)
6. sd_DATE comments (adds date and description on the head of the plot)
7. save **symdddzz.asc** (where y = year; ddd = day; zz = dye #)

- Edit **ne set-all.e** (code to correct single shots for dye curve and background subtraction) code:

- **Export file_app =**
 - g** = narrow-band dye laser background
 - f** = flame background
 - b** = camera noise background
 - fo** = offset background (average from baseline)
- **DYE=**
 - xx** = number of the run of the dye curve is in use for correction

```

set-all.e
File Edit Search Preferences Shell Macro Windows Help

# set-all.e 28-Mar-00
# alle wichtigen Uebergabeparameter werden jetzt "exportiert", damit nicht
# mehr soviel uebergeben werden muessen.
#
#-----
# Version 2.0 19-Apr-2000
# Version 2.1 20-Apr-2000
# Version 2.2 18-Jul-2000
# "export" ist wohl gar nicht noetig?!
# 12-Jun-2012 change in lfit.e: FILE_APP taken from $2 and RESAPP=${FILEAPP}${RES_APP}
#
# Leerstrings mit "xx" kennzeichnen!!!
#-----
# fuer korskp-ep.e:
export FILE_APP="g"
if [ "${FILE_APP}" = "bo" ] ; then KORSP_=" BLO KORR_OFF xx " ; fi
if [ "${FILE_APP}" = "b" ] ; then KORSP_=" BLO xx xx " ; fi
if [ "${FILE_APP}" = "f" ] ; then KORSP_=" FLA xx xx " ; fi
if [ "${FILE_APP}" = "fo" ] ; then KORSP_=" FLA KORR_OFF xx " ; fi
if [ "${FILE_APP}" = "fog" ] ; then KORSP_=" FLA KORR_OFF KORR_532 " ; fi
if [ "${FILE_APP}" = "g" ] ; then KORSP_=" 532 xx xx " ; fi
if [ "${FILE_APP}" = "go" ] ; then KORSP_=" 532 KORR_OFF xx " ; fi
DYE=05
AFILE0=${FILE_APP}
export FILE_APP=${FILE_APP}d${DYE}
AFILE=${FILE_APP}
# Schalter und Start und Endwert fuer spezielle Korrekturen:
export IF_KORR_AMAX="" # "" aktiv, "!" nicht aktiv
export IF_KORR_AMIN=""
export AMAX_V=60000 # filter value (saturation, breakdown, etc...)
export AMAX_N=0 # number of spectra to delete
export AMAX_S=70 # start pixel
export AMAX_E=120 # end pixel
export AMIN_V=-200 # Threshold to filter spectra with low values
export AMIN_S=75 # Threshold is checked in the
export AMIN_E=85 # average of this pixel range
export GRE_S=10
export GRE_E=30
export GRE2_S=220
export GRE2_E=250
export OFF_S=1 # When chosen Bkg "fo", these options set the range of pixels
export OFF_E=30 # where the average Bkg from baseline is calculated

# fuer all-ep.e
export R_KORSP="1"
export R_LFIT="1"
export R_SHOW="1"
export R_FINAL="0"
export MAXERR_LIST="50 40 30 25 20"

# Allgemeines:
export SHIFT=0,0
export ZOFF=false
export ZOFF=true

# fuer lfit.e:
# normale Auswertung:
export RES_APP=${FILE_APP}_1
export QFLIB="xx"
export LFLIB="xx"
export TAB_APP="${RES_APP}"
export KONSHIFT=1
export ICHNF=180
export ICHN=27
export ICHN_ADD=-29

export CHANNEL_A=1
export CHANNEL_B=${ICHNF}
export FACTOR_A=1,0
export FACTOR_B=1,0
export FACTOR_C=1,0
    
```

or "b","f","fo"

Threshold to filter spectra exceeding this value

saturation, breakdown, etc...

Threshold is checked in the

average of this pixel range

Threshold to filter spectra with low values

Threshold is checked in the

average of this pixel range

When chosen Bkg "fo", these options set the range of pixels where the average Bkg from baseline is calculated

```

# nur Hot-Band:
# export RES_APP=${FILE_APP}hbs
# export LFLIB="_hb"
# export TAB_APP="_3_${RES_APP}"
# export KONSHIFT=0
# export ICHNF=120
# export ICHN=88
# export ICHN_ADD=50

# Variables for lfit.e, qlib_nls.e und lflib_nls.e (parameter for different flames):
if [ "${LFLIB}" = "xx" ] ; then
export LFIT_P="4,935"
export LFIT_CONC="78,8426"
export LFIT_S_CONC="-0,00247529"
export LFIT_MIN_CONC="72,8"
export LFIT_MAX_CONC="78,1"
export LFIT_AXNRS="7,103"
export LFIT_S_AXNRS="0,000555294"
export LFIT_MIN_AXNRS="7,27"
export LFIT_MAX_AXNRS="8,45"
export LFIT_CONH2O="-0,01756235"
export LFIT_S_CONH2O="0,00005854"
export LFIT_MAX_CONH2O="0,1244"
export LFIT_CONCO2="-0,01608"
export LFIT_S_CONCO2="0,00005360"
export LFIT_MAX_CONCO2="0,1139"
fi

# fuer show*.et
export MAXERR=25
export METHOD=29
NEW=new
APP=app

# Spreadtest:
export DT="xx"
export M1="xx"
export M2="xx"
export M3="xx"
export SPREADTEST=" ${DT} ${M1} ${M2} ${M3} "
# -----

FLAMME="FIRST-III Referenzflamme"

#
EXP_06=" 06 ${AFILE} ${DYE} 0 107 FIRST-III 41 50 ${KORSP_} ${NEW} "
EXP_07=" 07 ${AFILE} ${DYE} 0 107 FIRST-III 38 50 ${KORSP_} ${APP} "
EXP_08=" 08 ${AFILE} ${DYE} 0 95 FIRST-III 32 50 ${KORSP_} ${APP} "
EXP_09=" 09 ${AFILE} ${DYE} 0 80 FIRST-III 22 50 ${KORSP_} ${APP} "
EXP_10=" 10 ${AFILE} ${DYE} 0 62 FIRST-III 35 50 ${KORSP_} ${APP} "
EXP_11=" 11 ${AFILE} ${DYE} 0 45 FIRST-III 35 50 ${KORSP_} ${APP} "
EXP_12=" 12 ${AFILE} ${DYE} 0 37 FIRST-III 41 50 ${KORSP_} ${APP} "
EXP_13=" 13 ${AFILE} ${DYE} 0 37 FIRST-III 41 50 ${KORSP_} ${APP} "
EXP_14=" 14 ${AFILE} ${DYE} 0 30 FIRST-III 38 50 ${KORSP_} ${APP} "
EXP_15=" 15 ${AFILE} ${DYE} 0 24 FIRST-III 44 50 ${KORSP_} ${APP} "
EXP_16=" 16 ${AFILE} ${DYE} 0 18 FIRST-III 48 50 ${KORSP_} ${APP} "
EXP_17=" 17 ${AFILE} ${DYE} 0 12 FIRST-III 55 50 ${KORSP_} ${APP} "
EXP_18=" 18 ${AFILE} ${DYE} 0 3 FIRST-III 10 50 ${KORSP_} ${APP} "
EXP_19=" 19 ${AFILE} ${DYE} 0 1 FIRST-III 8 50 ${KORSP_} ${APP} "
EXP_20=" 20 ${AFILE} ${DYE} 0 80 FIRST-III 28 50 ${KORSP_} ${APP} "

# Einstellungen fuer individuelle Namelists
#   SpekNr BKG T ConN2 ConH2O ConCO2 AXNRS PRESS
# NLS_04=" 04 ${AFILE} 1600,00 54,50 0,051 0,017 8,12 0,987"

# Kommentarstrings, die via gr.e in die Ausdrucke eingebunden werde
# ACHTUNG: Keine Leerzeichen im String verwenden !!

# GR_07="TLC_1bar_Phi=2,1_r=0mm_h=5mm_Gain=90"

```

The best way to check if the correction of the background and dye curve is correct is try to correct a room temperature spectrum. To do so, run **korsp-rt.e** program:

- **korsp-rt.e [room temperature run #] [dye curve run #]**

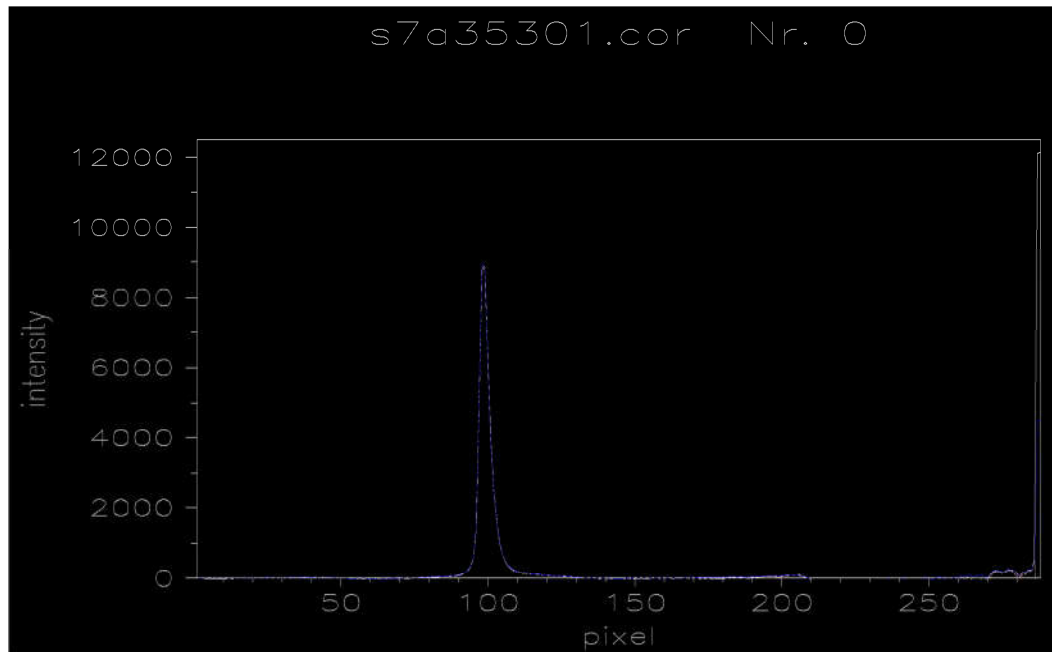
e.g. korsp-rt.e 01 04

The program has he following outputs:

- **xxayyy.cor** corrected averaged room temperature spectrum (carp format)

- `xxayy.sd` normalized, averaged room temperature spectrum (ASCII format)
- `xxuyy.asc` background for room temperature spectrum (ASCII format)

To visualize the resulting spectrum use `spi` (e.g. `spi -> chd xxayyy.cor -> gin`).

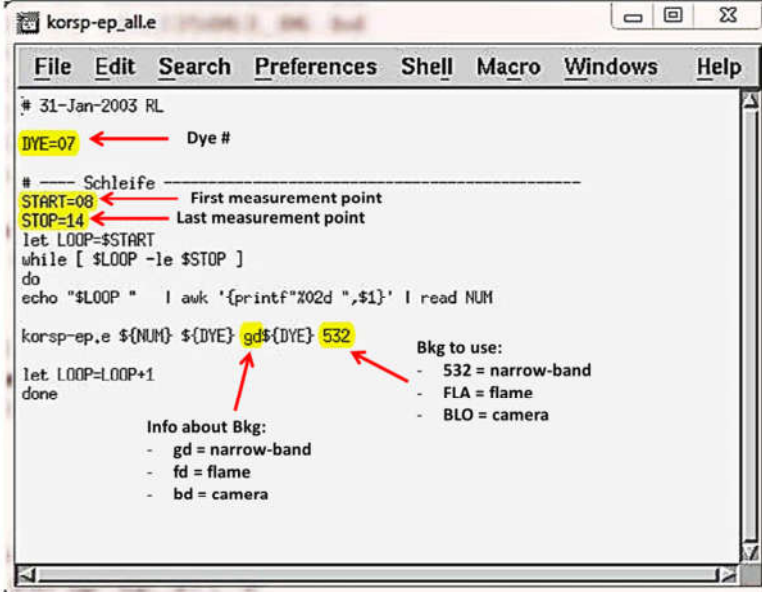


Repeat this procedure for all the room temperature spectra: the outputs of this program will be the inputs for the slit function calculation (see section 3).

After choosing the appropriate background and dye curve, save the changes and run **`korsp-ep.e [run#] [dye#] [bkg information to filename] [bkg]`** code to process one single shot

- e.g. `korsp-ep.e 03 99 fd99 FLA`

or **`korsp-ep_all.e`** (define the starting and ending point) to process all the data files (it calls `korsp-ep` for each single shot).



```

# 31-Jan-2003 RL
DYE=07 ← Dye #

# --- Schleife
START=08 ← First measurement point
STOP=14 ← Last measurement point
let LOOP=$START
while [ $LOOP -le $STOP ]
do
echo "$LOOP " | awk '{printf"%02d ",$1}' | read NUM

korsp-ep.e ${NUM} ${DYE} gd${DYE} 532

let LOOP=LOOP+1
done

Info about Bkg:
- gd = narrow-band
- fd = flame
- bd = camera

Bkg to use:
- 532 = narrow-band
- FLA = flame
- BLO = camera

```

The code provides the following outputs:

- **xxsyyyfd.cor** corrected of single CARS spectra
- **xxayyfd.cor** corrected averaged CARS spectrum (mmf format)
- **xxayyfd.sd** corrected averaged CARS spectrum (carp format)
- **xxayyfd.acs** corrected averaged CARS spectrum (ASCII format)
- **xxayyfd_.mmf** contains 10 spectra for procedure summary and check
 1. narrow-band dye laser background (532)
 2. broad-band dye laser background
 3. flame luminosity (laser off) background (FLA)
 4. averaged spectrum with complete dye curve correction
 5. averaged spectrum with offset correction (special correction)
 6. averaged spectrum with (special) correction for narrow-band
 7. averaged spectrum with camera linearity correction (not applicable for FlameStar2 camera)
 8. averaged spectrum after filter for minimum values is applied
 9. averaged spectrum after filter for maximum values is applied
 10. averaged spectrum with background (and 1-2 pixels) subtraction

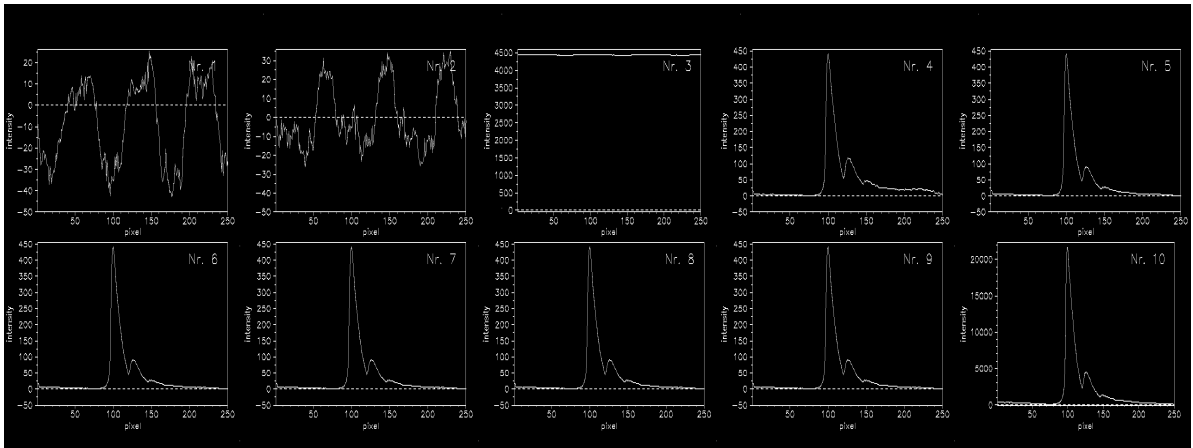
e.g. To visualize the summary spectra use the following command sequences:

1. spi
2. chd xxayyfd_.mmf
3. @spek
4. gino

Or in a different (and simpler) way you can use the **dis-bkg.e** command:

- **dis-bkg.e [name of corrected spectrum] ([ymin][ymax] optional)**

e.g. dis-bkg.e 10fd99 0 500



3. Calculation of the slit function

- Work in **apfit** folder
- The slit function is calculated in two steps; the first one involved the use of the room temperature spectrum recorded with the smaller slit width (usually 50 μ m, files are named with _50). The optimization involved the Lorentzian and Gaussian part of the slit function, and later the trapezoid part. The second part involved the room temperature spectrum recorded with a larger slit width (400 μ m, file are named with _1). The optimization involved mostly the middle part of the trapezoid, leaving almost constant the previously found parameters. The quality of the fit is determined mostly by looking and the comparison fit to data and by the F(Sum) error parameter. Usually a value of F(Sum)<0.2 is an indication of a good fit but it is not a strict rule.
- Edit the name-list file **ne standyyy_x.nls** (file containing all the inputs for fitting). Remember to rename the name-list file with the current day number (yyy):
 - **ICHN** = number of pixels to fit (default 80)
 - **ICHNO** = starting pixel point (default 50) for the fit: everything before is ignored
 - **RMAX** = maximum wavenumber (calculated by shift parameter)
 - **RMIN** = minimum wavenumber (useless if ICHN and ICHNO are in use)
 - **DISP** = dispersion of pixels (default 0.709)
 - **CHDISP** = non-linear dispersion (may be useful if DIS is not working by its own)
 - **KON_** = control variables for fit: 1=on, 0=off. Values aside are used as constant (KON=0) or starting values for fit (KON=1)
 - **SG** = Gaussian part of the slit (instrument) function
 - **SL** = Lorentzian part of the slit (instrument) function
 - **G1** = narrow-band dye laser linewidth
 - **DLL1** = narrow-band dye laser wavelength
 - **TRAPL** = trapezoid left part
 - **TRAPM** = trapezoid middle part
 - **TRAPR** = trapezoid right part
 - **ZTRAPLR** = symmetric trapezoid
 - **ZLORT** = Lorentzian part of the trapezoid
 - **ZPOSTCON** = postconvolution
 - **AXNRS** = non-resonant background (use 7.27 for air, otherwise use Gaseq software to calculate the chemical equilibrium at desired temperature and calculate the new value through the CARS_auswertung excel file)
 - **ZLIB** = creates libraries if true (T) (use it only after optimization)
 - **ZOFF** = fits for offset (use it only as last attempts if the background is very noisy)
 - **MAXF** = maximum iterations (remember that the error depends also on starting value)
 - **ACCREL** = relative accuracy (0.1 is a good value)
 - **IREFNO** = reference number (not used in the calculations, use the number of the day as identification)
 - **ZLOW** = collisional narrowing model for high pressure (p>3 atm) if T; otherwise uses model for low pressure (p<3 atm) when F.

```

stand137_1_50.nls
File Edit Search Preferences Shell Macro Windows Help
: &NDN
 ICHN = 80, ICHNO = 56,
 RMAX = 2344.174, RMIN = 2100.000,
 DISP = 0.7090000, CHDISP = 0.0000,
 DLMIN = 518.000000, DLMAX = 530.00000,
 KONGSHF = 1, SHIFT = 0.0000,
 KONT = 1, T = 294.0,
 KONTR = 0, TR = 300.0, ZTR = F,
 KONP = 0, P = 0.955,
 KONC = 0, CONC = 78.09,
 KONGSG = 0, SG = 0.734,
 KONGSL = 0, SL = 0.223,
 KONG1 = 0, G1 = 0.2500,
 DLL1 = 596.00000,
 ZPOSTCON = T, ZTRAPLR = F, ZLORT = T,
 KONTRAPL = 0, TRAPL = 0.000,
 KONTRAPM = 0, TRAPM = 0.000,
 KONTRAPR = 0, TRAPR = 0.235,
 AXNRS = 7.27E-18,
 CONH2O = 0.0000, CONCO2 = 0.0000,
 ZLIB = F, ZL = F, ZTRANS = T,
 ZOFF = F, ZO = T, ZSAME = F,
 ZR = F, ZSQRT = F,
 ZXC = T, ZXCA = T, ZLOW = T,
 ZX = F, ZVDPHA = T,
 KONSAS = 0, SAS = 0.0000,
 ALPHA2 = 3.2402E-51, RHO = 0.022000,
 THETA = 0.000, PHI = 0.0000,
 VDPHAS = 0.0000, XCDE = 1.0000,
 IP = -1, IPV = 0,
 MAXF = 50,
 ACCREL = 0.100, ACC = 0.000, HH = 0.000,
 IREFNO = 137, ITEST = 0
 /

```

- Edit **ne carp-rt_all.e** (program for room temperature fitting):
 - **NUM1** = number of run of room temperature spectrum (50 for 50 μ m, 1 for 400 μ m slit width)
 - **NLS** = number of namelist (.nls) file in use (**50** for 50 μ m, **1** for 400 μ m slit width)

```

carp-rt_all.e
File Edit Search Preferences Shell Macro Windows Help
# -----
# load variable definitions:
# ../mess/set.e
# -----
SPECSD1=${PRE}a${TAG}
KOMPAKT=kompakt.res
# -----
#
# No. of RT-spectra
NUM1=03
NUM2=-1
NUM3=-1
# No. of namelist to use
NLS=1
# -----
if [ $# -ge 1 ] ; then
    DUMMY=$1
else
    echo "use: $0 <run number> [<text for kompakt>]"
    exit
fi
# NUM=$3
# -----
echo " -${1}-${2}-----" >>${DIRAPFIT}${KOMPAKT}
echo " ${SPECSD1}${NUM1};" >>${DIRAPFIT}${KOMPAKT}
carp-rt.e ${NUM1} ${NLS} ecs $1 $2
# -----
if [ ${NUM2} -ne "-1" ] ; then
    echo " ${SPECSD1}${NUM2};" >>${DIRAPFIT}${KOMPAKT}
    carp-rt.e ${NUM2} ${NLS} ecs $1 $2
fi
# -----
if [ ${NUM3} -ne "-1" ] ; then
    echo " ${SPECSD1}${NUM3};" >>${DIRAPFIT}${KOMPAKT}
    carp-rt.e ${NUM3} ${NLS} ecs $1 $2
fi
# -----
#
#
#

```

Run the code:

- o **carp-rt_all.e [fit trial #] [optional comments (useful to track the fitting changes & parameters)]**

e.g. carp-rt_all.e 01 Fit:shift (2234)

This code creates the following outputs:

- o **file_01.bd** Fitted spectra and residue (binary, carp-format)
- o **file_01.zd** Fit information (all the iterations performed)
- o **kompakt.res** List of selected parameters for the fit

Verify the goodness of the fit by minimizing **F(Sum)** parameter.

```

-103-----
s6a32616:
  SG   SL  TRAPL  TRAPM  TRAPR  CONC   P    T    RMAX  CNT  FSUM  YMAX
1.378 .281 .015   .003   .303  78.09  1.0  300.0  2355.001  44  .8222 10865
1.378 .281 .014   .003   .306  78.09  1.0  300.0  2354.999  43  .8060 10689
1.378 .281 .002   .003   .302  78.09  1.0  300.0  2354.990  34  .7443 10706

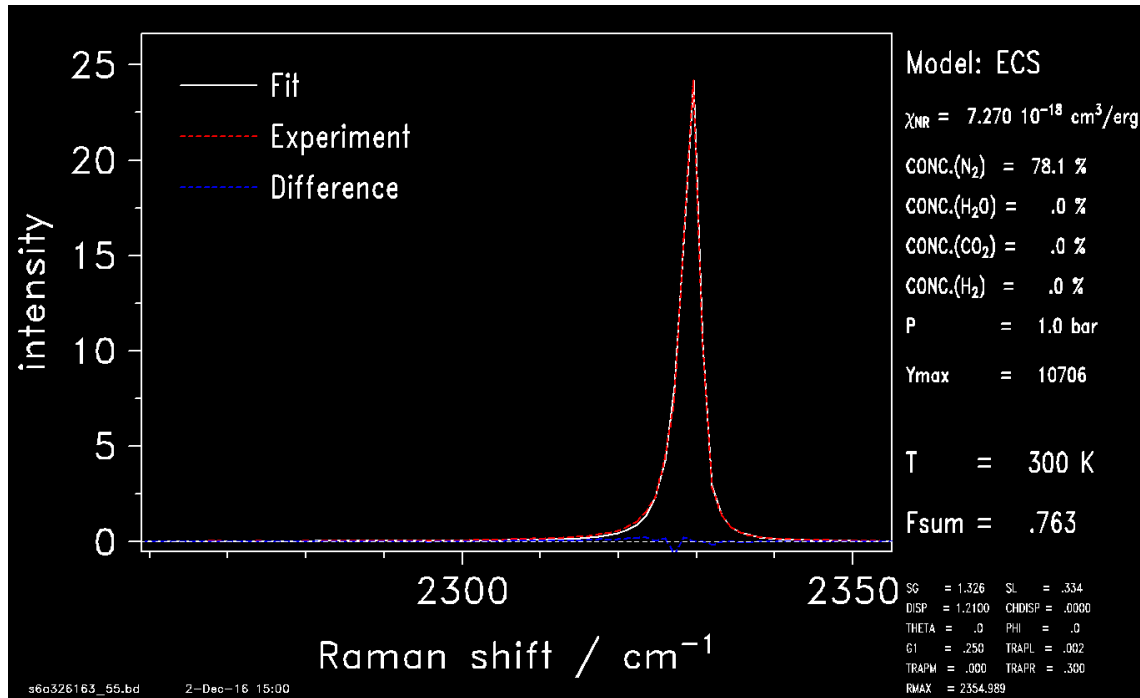
```

Then check the the goodness of the fit by looking at theory to data plot using **gr.e** program:

- o **gr.e [room temperature run #]_[fit trial #]**

e.g. gr.e 3314_01

(note: a black window pops up: double-click on mouse middle button to activate the plot)



Iterate fitting the room temperature spectra using the following procedure:

1. Start with room temperature spectrum with 50 μm slit width.
2. Fit only for horizontal shift (KONSHF=1, every other KON variable = 0, temperature fixed at measured room temperature value).
3. Update the starting value of the shift modifying ICNH0 value based on R_MAX fit.
4. Fit for Gaussian (SL=1) and Lorentzian (SG=1) part of the slit function coupled with horizontal shift (with updated ICNH0 starting value); keep TRAPM = 0.
5. Remove SL(=0) and SG(=0) from the fitting parameter (updating the values to the best fit) and activate left (TRAPL=1) and right (TRAPR=1) trapezoid part.
6. Fit one last time only for temperature (to verify the value of measured room temperature).
7. Switch to room temperature spectrum with 400 μm slit width and edit the carp_rt_all.e according to the new inputs.
8. Keep all the updated fitting values from the 50 μm fit.
9. Activate only middle (TRAPM=1) trapezoid part and fit for it.
10. Once updated the value, fir only for TRAPL and TRAPR.
11. Last fit with only temperature again.

4. Calculation of dispersion

- If the spectra are not all corrected for background subtraction and dye curve, go to **mess** folder.
- Process a hot spectrum subtraction the background (**korsp-nr.e** code) and correcting for dye curve (**korsp-ep.e** code). Detailed instructions are provided in previous section 2.
- Copy **carp** folder from previous data analysis folder if it is not present
- Now work in **carp** folder.
- Edit **ne carp-fit_all.e**
 - **AFILE = "gdxx"** where xx is the value in the name-file of **.sd** output in mess folder
 - **NUM=xx\${AFILE}** where xx is the run number of the hot spectrum to fit

```

carp-fit_all.e
File Edit Search Preferences Shell Macro Windows Help
# 27-Nov-2001: namelist now carp${TAG}_x.nls
#
# load variable definitions:
# ../mess/set.e
#
SPECSD1=${PRE}a${TAG}
MODEL=ecs
KOMPAKT=kompakt,res
if [ ! $# -ge 2 ] ; then
  echo "use: $# <run number> <text for kompakt,res> <number of exp.,> <NLS number>"
  exit
else
#
# create namelist files for different phi's:
NLS=carp${TAG}_
#NLS0=${NLS}1.nls
#
AFILE="gd13"
#
echo "${1} -- ${2} -----" >>${KOMPAKT}
#
#
if [ $# -ge 4 ] ; then
  NUM=$3
  NLS_NUM=$4
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} ${NLS_NUM} ${MODEL} $1 $2
  exit
fi

if [ 1 -eq 1 ] ; then
  AFILE="gd13"
#
  NUM=07${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 100 ${MODEL} $1 $2
#
fi

if [ 1 -eq 0 ] ; then
#
  NUM=04${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=05${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=06${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=07${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=08${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=11${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=12${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#
  NUM=13${AFILE}
  echo "${SPECSD1}${NUM}_${1}" >>${KOMPAKT}
  carp-fit.e ${NUM} 1 ${MODEL} $1 $2
#

```

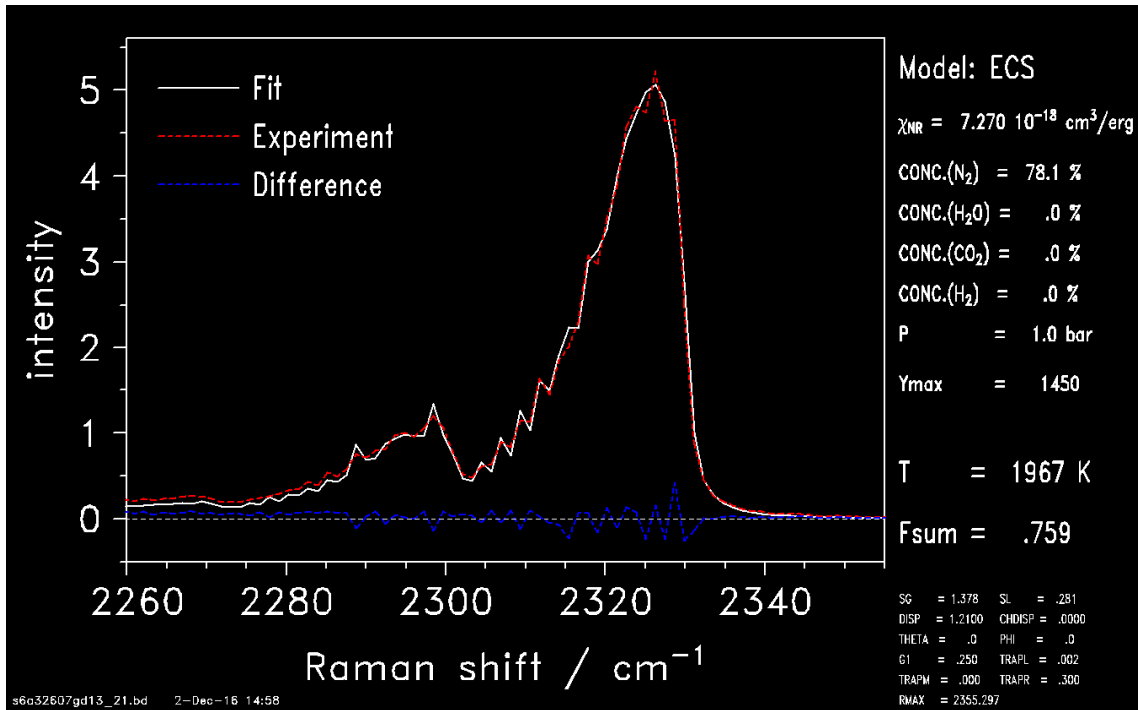
- Using the previous found slit function parameters, fit the hot spectrum for temperature first (**KONT = 1**) and then for dispersion (**DISP**) modifying the **carpxxx_100.nls**. Remember to modify **ZLOW = (T for p < 1.5 atm or F for p > 1.5 atm)**.

```

File Edit Search Preferences Shell Macro Windows Help
&NDN
ICHN = 80, ICHNO = 56,
RMAX = 2344.335, RMIN = 2100.000,
DISP = 0.7090000, CHDISP = 0.0000,
DLMIN = 518.000000, DLMAX = 530.000000,
KONSHF = 0, SHIFT = 0.0000,
KONT = 1, T = 294.0,
KONTR = 0, TR = 300.0, ZTR = F,
KONP = 0, P = 0.955,
KONC = 0, CONC = 78.09,
KONSG = 0, SG = 0.734,
KONSL = 0, SL = 0.223,
KONG1 = 0, G1 = 0.2500,
DLL1 = 596.00000,
ZPOSTCON = T, ZTRAPLR = F, ZLORT = T,
KONTRAPL = 0, TRAPL = 0.011,
KONTRAPM = 0, TRAPM = 2.100,
KONTRAPR = 0, TRAPR = 0.400,
AXNRS = 7.27E-18,
CONH2O = 0.0000, CONCO2 = 0.0000,
ZLIB = F, ZL = F, ZTRANS = T,
ZOFF = F, ZO = T, ZSAFE = F,
ZR = F, ZSQRT = F,
ZXC = T, ZXCA = T, ZLOW = T,
ZX = F, ZVDPHA = T,
KONSAS = 0, SAS = 0.0000,
ALPHA2 = 3.2402E-51, RHO = 0.022000,
THETA = 0.000, PHI = 0.0000,
VDPHAS = 0.0000, XCDE = 1.0000,
IP = -1, IPV = 0,
MAXF = 50,
ACCREL = 0.100, ACC = 0.000, HH = 0.000,
IREFNO = 137, ITEST = 0,
/

```

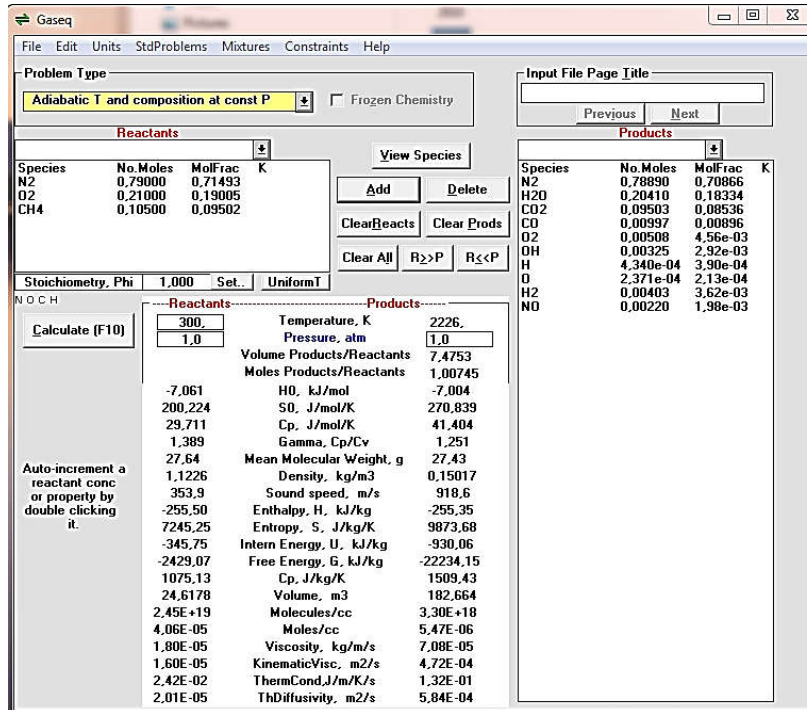
- Run **carp-fit_all.e**:
 - carp-fit_all.e [# of fit] [basenamefile of spectrum to fit] [.nls#]**
e.g. carp-fit_all.e 01 14fd99 100
- As for the slit function, first minimize the **F(sum)** and then check the goodness of the fit using the **gr.e** command.



The goal is to align all the rotational lines even if the F(sum) may increase. Once found the optimum dispersion value, repeat the slit function calculation (section 3) using the new updated dispersion value. Iterate again between dispersion and slit function until convergence is found.

5. Creation of quick fit library

- Work in **mess** folder.
- Before starting, run **gaseq** code and note all the specie concentrations for the tested flame at maximum temperature (at stoichiometric conditions, $\phi = 1$).



The screenshot shows the Gaseq software interface. The 'Problem Type' is set to 'Adiabatic T and composition at const P'. The 'Reactants' table lists N2, O2, and CH4 with their respective moles and mole fractions. The 'Products' table lists N2, H2O, CO2, CO, O2, OH, H, O, H2, and NO with their respective moles and mole fractions. The 'Stoichiometry, Phi' is set to 1.000. The 'Calculate (F10)' button is visible. The bottom section displays various thermodynamic and transport properties for the mixture.

Species	No. Moles	MolFrac	K
N2	0.79000	0.71493	
O2	0.21000	0.19005	
CH4	0.10500	0.09502	

Species	No. Moles	MolFrac	K
N2	0.78890	0.70866	
H2O	0.20410	0.18334	
CO2	0.09503	0.08536	
CO	0.00997	0.00896	
O2	0.00508	4.56e-03	
OH	0.00325	2.92e-03	
H	4.340e-04	3.90e-04	
O	2.371e-04	2.13e-04	
H2	0.00403	3.62e-03	
NO	0.00220	1.98e-03	

Reactants	Products
Temperature, K	2226.
Pressure, atm	1.0
Volume Products/Reactants	7.4753
Moles Products/Reactants	1.00745
H0, kJ/mol	-7.004
S0, J/mol/K	270.839
Cp, J/mol/K	41.404
Gamma, Cp/Cv	1.251
Mean Molecular Weight, g	27.43
Density, kg/m3	0.15017
Sound speed, m/s	918.6
Enthalpy, H, kJ/kg	-255.35
Entropy, S, J/kg/K	9873.68
Intern Energy, U, kJ/kg	-930.06
Free Energy, G, kJ/kg	-22234.15
Cp, J/kg/K	1509.43
Volume, m3	182.664
Molecules/cc	3.30E+18
Moles/cc	5.47E-06
Viscosity, kg/m/s	7.08E-05
KinematicVisc, m2/s	4.72E-04
ThermCond, J/m/K/s	1.32E-01
Thdiffusivity, m2/s	5.84E-04

Use those values to update the tables in the excel file **CARS_auswertung**.

First update the value for the fuel with all the product concentration in order to evaluate the maximum AXNRS:

#	A	B	C	D	E
1	JetA1-Air Flame				
2	Phi = 1,0				
3					
4	Moleküle	AXNRS	Konzentrationen	AXNRS	
5					
6	N ₂	7,10	73,067	5,188	
7	H ₂ O	15,50	12,134	1,881	
8	CO ₂	9,20	11,652	1,072	
9	CO	9,80	1,504	0,147	
10	O ₂	7,80	0,667	0,052	
11	H ₂	7,00	0,285	0,020	
12	Ar	9,60	0,000	0,000	
13	NO	18,90	0,276	0,052	
14	CH ₄	31,80		0,000	
15	C ₂ H ₄	84,90		0,000	
16	C ₃ H ₆	126,70		0,000	
17	C ₄ H ₈	147,80		0,000	
18	i-C ₄ H ₁₀	130,60		0,000	
19					
20	Summe:		99,585	8,412	
21					

Then update also the table in tab **T-Abhängigkeiten** and note all the values inside: they will be the inputs to for the library creation.

		T-kalt		N ₂ -kalt		min_axnrs														
CARS-Exp.	Flamme	p	Φ	T-heiB-Tad	N ₂ -0 conc	N-T u_conc	N2-heiB min_conc	N2-kalt max_conc	AXNRS-0 axnrs	AXNRS-T u_axnrs	AXNRS-heiB max_axnrs	H2O-0 con_h2o	H2O-T u_conh2o	H2O-heiB max_conh2o	CO2-0 con_co2	CO2-T u_conco2	CO2-heiB max_conco2	H2-0 con_h2	H2-T u_conh2	H2-heiB max_conh2
	Flamme-I	3%	0,86	2264	76,7263	-0,00209758	76,0	78,1	7,160020	0,000366599	7,99	-0,01680344	0,00005601	0,11	-0,01680344	0,00005601	0,11	-0,02206703	0,00007352	0,1444
	Flamme-II	3%	1,2	1726	78,8628	-0,00154278	75,9	78,1	7,147989	0,000408732	7,85	-0,01577840	0,00005259	0,075	-0,01577840	0,00005259	0,075	-0,01037868	0,00019126	0,1444
	Flamme-III	4%	0,87	1855	78,8596	-0,00186409	75,2	78,1	7,194759	0,000250404	7,66	-0,01717842	0,00005123	0,089	-0,01717842	0,00005123	0,089	-0,02786652	0,00009296	0,1444
	Flamme-IV	3%	0,64	1886	78,8107	-0,00170240	75,4	78,1	7,235145	0,00018285	7,56	-0,01607818	0,00005359	0,085	-0,01607818	0,00005359	0,085	-0,02731408	0,00009105	0,1444

Note that all the species (H₂O, CO₂, H₂) must be written in absolute mole fraction except N₂ which must be written in percentage.

- Edit the **ne set.all.e** program: update all the values about the slit function obtained in the previous section and update all the values regarding the specie concentrations, maximum and minimum values, non-resonant background, pressure and the values of the slopes. The last information are obtained from the excel sheet. Regarding the method, use the 29. It is proved to be best one (however, after fitting it is possible to compare different methods and choose the most appropriate one if 29 is not satisfactory).

```

set-alle
File Edit Search Preferences Shell Macro Windows Help
# set-all.e 28-Mar-00
# alle wichtigen Uebergabeparameter werden jetzt "exportiert", damit nicht
# mehr soviel uebergeben werden muessen.
# -----
# Version 2,0 19-Apr-2000
# Version 2,1 20-Apr-2000
# Version 2,2 18-Jul-2000
# "export" ist wohl gar nicht noetig?!
# 12-Jun-2012 change in lfit.e: FILE_APP taken from $2 and RESAPP=${FILEAPP}${RES_APP}
# -----
# Leerstrings mit "xx" kennzeichnen!!!
# -----
# fuer korsk-ep.e:
export FILE_APP="g"
if [ "${FILE_APP}" = "bo" ] ; then KORS_=" BLO KORR_OFF xx " ; fi
if [ "${FILE_APP}" = "b" ] ; then KORS_=" BLO xx xx " ; fi
if [ "${FILE_APP}" = "f" ] ; then KORS_=" FLA xx xx " ; fi
if [ "${FILE_APP}" = "fo" ] ; then KORS_=" FLA KORR_OFF xx " ; fi
if [ "${FILE_APP}" = "fog" ] ; then KORS_=" FLA KORR_OFF KORR_532 " ; fi
if [ "${FILE_APP}" = "g" ] ; then KORS_=" 532 xx xx " ; fi
if [ "${FILE_APP}" = "go" ] ; then KORS_=" 532 KORR_OFF xx " ; fi
DYE=05
AFILE0=${FILE_APP}
export FILE_APP=${FILE_APP}d${DYE}
AFILE=${FILE_APP}
# Schalter und Start und Endwert fuer spezielle Korrekturen:
export IF_KORR_AMAX="" # "" aktiv, != "" nicht aktiv
export IF_KORR_AMIN=""
export AMAX_V=60000 # filter value
export AMAX_N=0 # number of spectra to delete
export AMAX_S=70 # start pixel
export AMAX_E=120 # end pixel
export AMIN_V=-200
export AMIN_S=75
export AMIN_E=85
export GRE_S=10
export GRE_E=30
export GRE2_S=220
export GRE2_E=250
export OFF_S=1
export OFF_E=30

# fuer all-ep.e
export R_KORS="1"
export R_LFIT="1"
export R_SHOW="1"
export R_FINAL="0"
export MAXERR_LIST="50 40 30 25 20"

# Allgemeines:
export SHIFT=0,0
export ZOFF=false
# export ZOFF=true

# fuer lfit.e:
# normale Auswertung:
export RES_APP=${FILE_APP}_1
export QFLIB="xx"
export LFLIB="xx"
export TAB_APP=${RES_APP}
export KONSHIFT=1
export ICHNF=180
export ICHN=27
export ICHN_ADD=-29

export CHANNEL_A=1
export CHANNEL_B=${ICHNF}
export FACTOR_A=1.0
export FACTOR_B=1.0

```

```

# nur Hot-Band:
# export RES_APP=${FILE_APP}hbs
# export LFLIB="_hb"
# export TAB_APP="_3_${RES_APP}"
# export KONSHIFT=0
# export ICHNF=120
# export ICHN=88
# export ICHN_ADD=50

# Variables for lfit.e, qflib_nls.e und lflib_nls.e (parameter for different flames):
if [ "${LFLIB}" = "xx" ]; then
export LFIT_P="4.935"
export LFIT_CONC="78.8426"
export LFIT_S_CONC="-0.00247525"
export LFIT_MIN_CONC="72.8"
export LFIT_MAX_CONC="78.1"
export LFIT_AXNRS="7.103"
export LFIT_S_AXNRS="0.000555254"
export LFIT_MIN_AXNRS="7.27"
export LFIT_MAX_AXNRS="8.45"
export LFIT_CONH2O="-0.0175623"
export LFIT_S_CONH2O="0.00005854"
export LFIT_MAX_CONH2O="0.1244"
export LFIT_CONCO2="-0.01608"
export LFIT_S_CONCO2="0.00005360"
export LFIT_MAX_CONCO2="0.1139"
fi

# fuer show*.e:
export MAXERR=25
export METHOD=29
NEW=new
APP=app

# Spreadtest:
export DT="xx"
export M1="xx"
export M2="xx"
export M3="xx"
export SPREADTEST=" ${DT} ${M1} ${M2} ${M3} "
# -----
FLAME="FIRST-III Referenzflamme"

#
# r HAB F1. 532 BB
EXP_06=" 06 ${AFILE} ${DYE} 0 107 FIRST-III 41 50 ${KORSP_} ${NEW} "
EXP_07=" 07 ${AFILE} ${DYE} 0 107 FIRST-III 38 50 ${KORSP_} ${APP} "
EXP_08=" 08 ${AFILE} ${DYE} 0 95 FIRST-III 32 50 ${KORSP_} ${APP} "
EXP_09=" 09 ${AFILE} ${DYE} 0 80 FIRST-III 22 50 ${KORSP_} ${APP} "
EXP_10=" 10 ${AFILE} ${DYE} 0 62 FIRST-III 35 50 ${KORSP_} ${APP} "
EXP_11=" 11 ${AFILE} ${DYE} 0 45 FIRST-III 35 50 ${KORSP_} ${APP} "
EXP_12=" 12 ${AFILE} ${DYE} 0 37 FIRST-III 41 50 ${KORSP_} ${APP} "
EXP_13=" 13 ${AFILE} ${DYE} 0 37 FIRST-III 41 50 ${KORSP_} ${APP} "
EXP_14=" 14 ${AFILE} ${DYE} 0 30 FIRST-III 38 50 ${KORSP_} ${APP} "
EXP_15=" 15 ${AFILE} ${DYE} 0 24 FIRST-III 44 50 ${KORSP_} ${APP} "
EXP_16=" 16 ${AFILE} ${DYE} 0 18 FIRST-III 48 50 ${KORSP_} ${APP} "
EXP_17=" 17 ${AFILE} ${DYE} 0 12 FIRST-III 55 50 ${KORSP_} ${APP} "
EXP_18=" 18 ${AFILE} ${DYE} 0 3 FIRST-III 10 50 ${KORSP_} ${APP} "
EXP_19=" 19 ${AFILE} ${DYE} 0 1 FIRST-III 8 50 ${KORSP_} ${APP} "
EXP_20=" 20 ${AFILE} ${DYE} 0 80 FIRST-III 28 50 ${KORSP_} ${APP} "

# Einstellungen fuer individuelle Namelists
# SpekNr BKG T CcnM2 ConH2O ConCO2 AXNRS PRESS
# NLS_04=" 04 ${AFILE} 1600,00 54,50 0,051 0,017 8,12 0,987"

# Kommentarstrings, die via gr.e in die Ausdrucke eingebunden werde
# ACHTUNG: Keine Leerzeichen im String verwenden !!

# GR_07="TLC_1bar_Phi=2.1_r=0mm_h=5mm_Gain=90"

```

- Now work in **qflib** folder.
- Rename (with the data day number) and edit the name-list file (**qflibxxx.nls**): update all the values about the slit function obtained in the previous section.

```

qflib137.nls
File Edit Search Preferences Shell Macro Windows Help
: &NDN
ICHN = 150, ICHNO = 55,
RMAX = 2344.440, RMIN = 2100.000,
DISP = 0.7050000, CHDISP = 0.0000,
DLMIN = 471.000000, DLMAX = 473.000000,
KONSHF = 0, SHIFT = 0.0000,
KONT = 0, T = 290.0,
KONTR = 0, TR = 300.0, ZTR = F,
KONP = 0, P = 4.935,
KONC = 0, CONC = 78.09,
KONSG = 0, SG = 0.734,
KONSL = 0, SL = 0.223,
KONG1 = 0, G1 = 0.2500,
DLL1 = 596.00000,
ZPOSTCON = T, ZTRAPLR = F, ZLORT = T,
KONTRAPL = 0, TRAPL = 0.011,
KONTRAPM = 0, TRAPM = 2.100,
KONTRAPR = 0, TRAPR = 0.400,
AXNRS = 7.27E-18,
CONH20 = 0.001, CONCO2 = 0.003, CONH2 = 0.0,
ZLIB = F, ZL = F, ZTRANS = T,
ZOFF = F, ZO = T, ZSAME = F,
ZR = F, ZSQRT = F,
ZXC = T, ZXCA = T, ZLOW = T,
ZX = F, ZVDPHA = T,
KONSAS = 0, SAS = 0.0000,
ALPHA2 = 3.2402E-51, RHO = 0.022000,
THETA = 0.000, PHI = 0.0000,
VDPHAS = 0.0000, XCDE = 1.0000,
IP = -1, IPV = 0,
MAXF = 50,
ZLOW = T for pressure < 1.5 atm
ZLOW = F for pressure > 1.5 atm

```

- Run **qflib_nls.e** program to create all the filename lists to generate the the library (.cnr file).
 - **qflib_nls.e**
 - This code creates the following outputs:
 - **.cnn** Large series for different temperatures (default every 50 K)
- Run **carp-qf.e** program to create the library through the already created .cnr filename list.
 - **carp-qf.e ""**

This code creates the following outputs:

- **.crl** Spectral library
- **.zd** Input/output parameters
- **output.log** Logfile with carp- errorlist
- **kompakt.res** Selective outputs

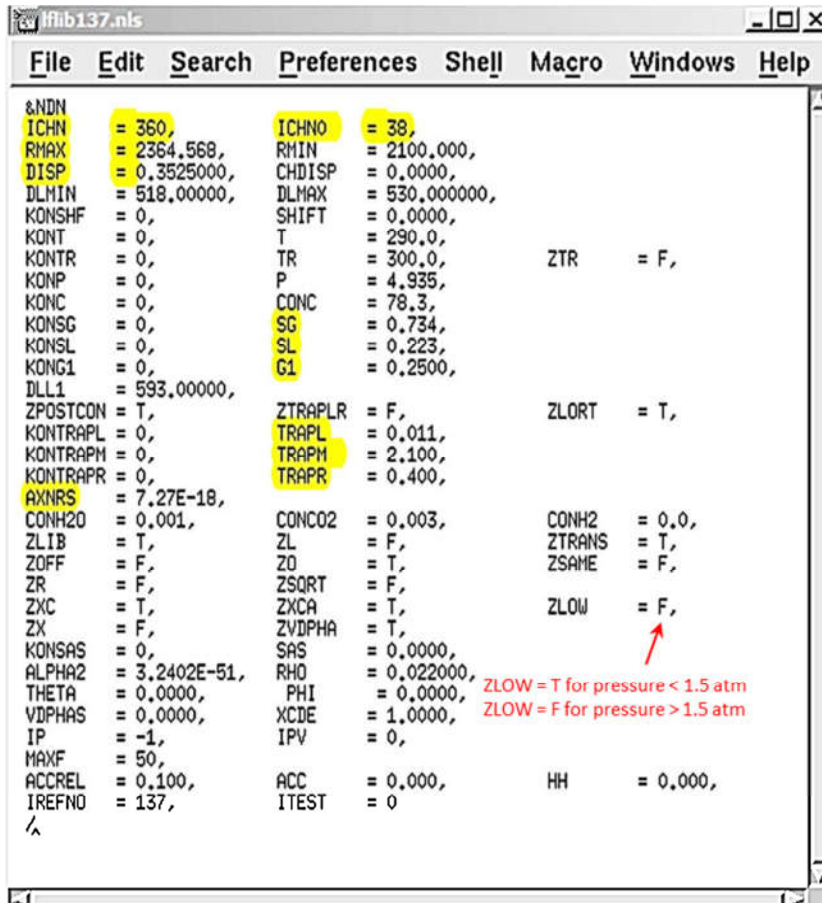
- Run **anal.e** program to analyze the the library coefficients and write them into a table
 - **anal.e ""**

This code creates the following outputs:

- **.cff** Input parameters
 - **.cft** Table with spectra
-
- Run **clean-ql.e** program to delete all the unnecessary file
 - **clean-ql.e**

6. Creation of fit library

- Work in **lflib** folder.
- Modify **lflibxxx.nls** accordingly to slit function and AXNRS values. Change the RMAX value taking into consideration that the quick fit library and the fit library are shifted by a certain amount of pixels (default value -30. This number is found in set-all.e file – mess folder – under ICHN_ADD variable). To align the two libraries **RMAX** value should be increased (or decreased) by the RMAX value of the quick fit library multiplied by the dispersion value: it is possible to find these numbers in the qflibxxx.nls file in qflib folder. Note also that the number of pixel to fit in the fit library is higher than the quick fit library (do not change **ICHN** value): this implies that the dispersion value (**DISP**) must be half of the one found in the quick fit library.

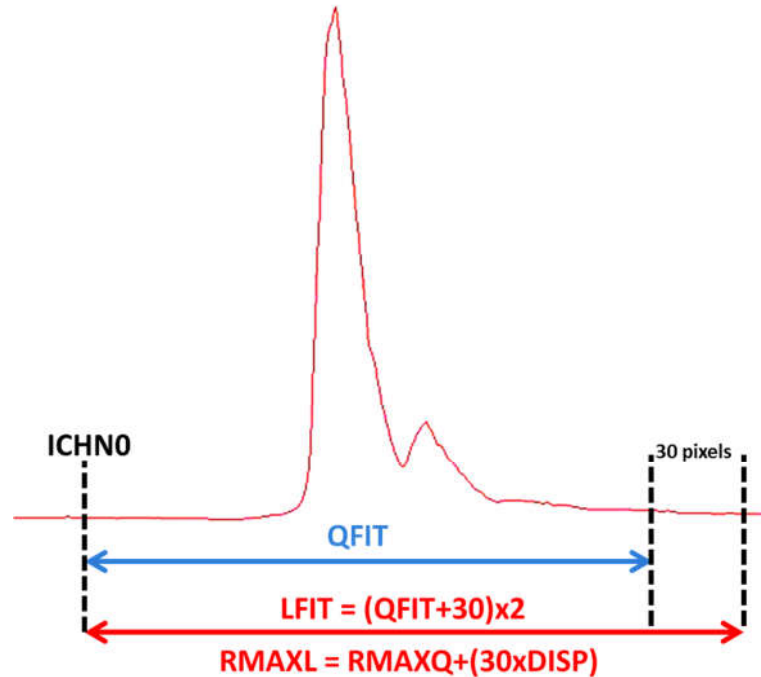


```

&NDN
ICHN = 360, ICHNO = 38,
RMAX = 2364.568, RMIN = 2100.000,
DISP = 0.3525000, CHDISP = 0.0000,
DLMIN = 518.00000, DLMAX = 530.000000,
KONSHF = 0, SHIFT = 0.0000,
KONT = 0, T = 290.0,
KONTR = 0, TR = 300.0, ZTR = F,
KONP = 0, P = 4.935,
KONC = 0, CONC = 78.3,
KONSG = 0, SG = 0.734,
KONSL = 0, SL = 0.223,
KONG1 = 0, G1 = 0.2500,
DLL1 = 593.00000,
ZPOSTCON = T, ZTRAPLR = F, ZLORT = T,
KONTRAPL = 0, TRAPL = 0.011,
KONTRAPM = 0, TRAPM = 2.100,
KONTRAPR = 0, TRAPR = 0.400,
AXNRS = 7.27E-18,
CONH2O = 0.001, CONCO2 = 0.003, CONH2 = 0.0,
ZLIB = T, ZL = F, ZTRANS = T,
ZOFF = F, ZO = T, ZSAME = F,
ZR = F, ZSQRT = F,
ZXC = T, ZXCA = T, ZLOW = F,
ZX = F, ZVDPHA = T,
KONSAS = 0, SAS = 0.0000,
ALPHA2 = 3.2402E-51, RHO = 0.022000,
THETA = 0.0000, PHI = 0.0000,
VDPHAS = 0.0000, XCDE = 1.0000,
IP = -1, IPV = 0,
MAXF = 50,
ACCREL = 0.100, ACC = 0.000, HH = 0.000,
IREFNO = 137, ITEST = 0
^

```

ZLOW = T for pressure < 1.5 atm
ZLOW = F for pressure > 1.5 atm



- Run **lflib_nls.e** program to create all the filename lists to generate the library (.cnr file).
 - **lflib_nls.e**
 - This code creates the following outputs:
- **.cnr** Large series for different temperatures (default every 50 K)
- Run **carp-lf.e** program to create the library through the already created .cnr filename list.
 - **carp-lf.e ""**
 - This code creates the following outputs:
- **.lib** Large spectral libraries for different temperatures
- Run **clean-lf.e** program to delete all the unnecessary file
 - **clean-lf.e**

A quick method to check if the two libraries are well aligned is to create some theoretical spectra (one every 50 K) using the QFit library and try to fit them using the LFit library. The initial temperature guess is set on purpose 200 K above the right temperature to force the LFit code to do some iterations. To do so, run the code **lfit_qlfit.e** in **lfit** folder. Results are found in **qflib** folder:

- **qflibxxx.dat**
- **qflibxxx.lft**
- **qflibxxx.log**
- **qflibxxx.res**

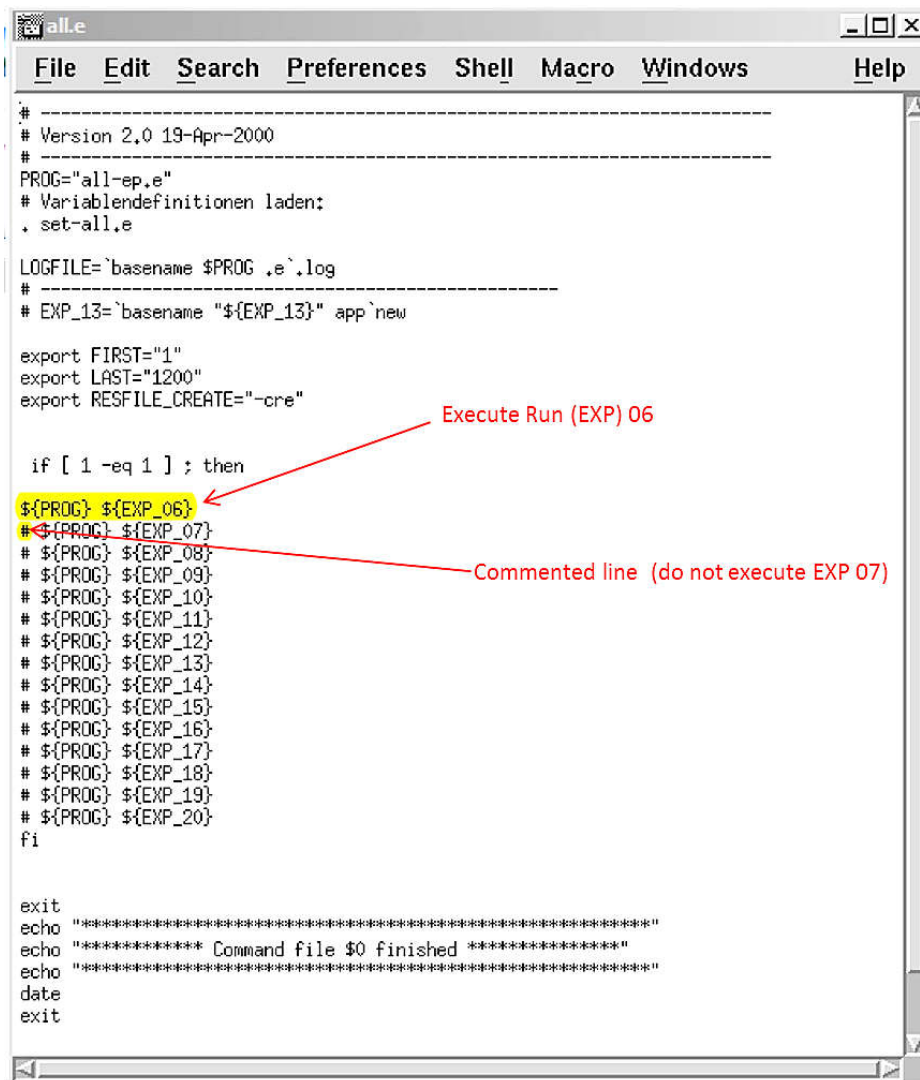
If the two libraries are well aligned the **F(Sum)** should be low and the temperatures very close. Check this on the **.log** file. Also, it is possible to see the fit using spi program:

1. spi
2. chd qflibxxx.lft
3. @fit
4. gin

7. Fit the spectra

- Work in **mess** folder
- Edit **ne all.e** program (code to enable the fit to all single shots of every data point – remember: each data point contains 1200 single shots).

All the lines with **#** are commented and not executed. **EXP_xx** is the data point followed by run number.



```

all.e
File Edit Search Preferences Shell Macro Windows Help
# -----
# Version 2,0 19-Apr-2000
# -----
PROG="all-ep.e"
# Variablendefinitionen laden:
. set-all.e

LOGFILE=`basename $PROG .e`.log
# -----
# EXP_13=`basename "${EXP_13}" app`new

export FIRST="1"
export LAST="1200"
export RESFILE_CREATE="-cre"

if [ 1 -eq 1 ] ; then
${PROG} ${EXP_06}
# ${PROG} ${EXP_07}
# ${PROG} ${EXP_08}
# ${PROG} ${EXP_09}
# ${PROG} ${EXP_10}
# ${PROG} ${EXP_11}
# ${PROG} ${EXP_12}
# ${PROG} ${EXP_13}
# ${PROG} ${EXP_14}
# ${PROG} ${EXP_15}
# ${PROG} ${EXP_16}
# ${PROG} ${EXP_17}
# ${PROG} ${EXP_18}
# ${PROG} ${EXP_19}
# ${PROG} ${EXP_20}
fi

exit
echo "*****"
echo "***** Command file $0 finished *****"
echo "*****"
date
exit

```

- Edit **ne set-all.e**:
 - **AMAX_V** = filter for too high intensity / camera saturation (maximim value)
 - **AMAXN** = # of spectra to delete
 - **AMAX_S** = start point (pixel #) where to apply the max filter
 - **AMAX_E** = end point (pixel #) where to apply the max filter
 - **AMIN_V** = filter for too low intensity / camera noise (minimum value)

- **AMIN_S** = start point (pixel #) where to apply the min filter
- **AMIN_E** = end point (pixel #) where to apply the min filter
- **R_KORSP** = correct spectra (bkg, dye curve) if = "1" (skip process if = "0")
- **R_LFIT** = fit spectra if = "1" (skip process if = "0")
- **R_SHOW** = show results (table) if = "1" (skip process if = "0")
- **R_FINAL** = summarize results and statistics if = "1" (skip process if = "0")
- **MAXERR_LIST** = maximum F(Sum) error to reject spectra in statistics
- **ICHNF** = # of pixels used to fit by fit library (lflib): 180 is default value
- **ICHN** = # of pixels skipped from data to library (use the same # used in standxxx_1.nls in apfit folder)
- **ICHN_ADD** = # of pixels added to match quick fit (smaller) to regular fit library

Remember to list all the run # in the experiment at the end of the program otherwise the code stops at the last EXP_xx. Also, it is possible to edit the measurement position modifying the values under the columns **r** (radial position) and **HAB** (height above burner).

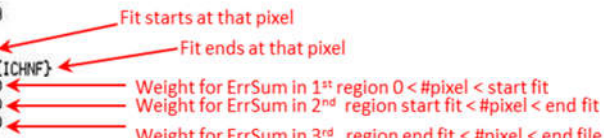
```

set-all.e
File Edit Search Preferences Shell Macro Windows Help
# set-all.e 28-Mar-00
# alle wichtigen Uebergabeparameter werden jetzt "exportiert", damit nicht
# mehr soviel uebergeben werden muessen.
# -----
# Version 2.0 19-Apr-2000
# Version 2.1 20-Apr-2000
# Version 2.2 18-Jul-2000
# "export" ist wohl gar nicht noetig?!
# 12-Jun-2012 change in lfit.e: FILE_APP taken from $2 and RESAPP=${FILEAPP}${RES_APP}
# -----
# Leerstrings mit "xx" kennzeichnen!!!
# -----
# fuer korsk-ep.e:
export FILE_APP="g"
if [ "${FILE_APP}" = "bo" ] > then KORS_P=" BLO KORR_OFF xx " ; fi
if [ "${FILE_APP}" = "b" ] > then KORS_P=" BLO xx xx " ; fi
if [ "${FILE_APP}" = "f" ] > then KORS_P=" FLA xx xx " ; fi
if [ "${FILE_APP}" = "fo" ] > then KORS_P=" FLA KORR_OFF xx " ; fi
if [ "${FILE_APP}" = "fog" ] > then KORS_P=" FLA KORR_OFF KORR_532 " ; fi
if [ "${FILE_APP}" = "g" ] > then KORS_P=" 532 xx xx " ; fi
if [ "${FILE_APP}" = "go" ] > then KORS_P=" 532 KORR_OFF xx " ; fi
DYE=05
AFILE0=${FILE_APP}
export FILE_APP=${FILE_APP}d${DYE}
AFILE=${FILE_APP}
# Schalter und Start und Endwert fuer spezielle Korrekturen:
export IF_KORR_AMAX="" # "" aktiv, "=" nicht aktiv
export IF_KORR_AMIN=""
export AMAX_V=60000 # filter value
export AMAX_N=0 # number of spectra to delete
export AMAX_S=70 # start pixel
export AMAX_E=120 # end pixel
export AMIN_V=-200
export AMIN_S=75
export AMIN_E=85
export GRE_S=10
export GRE_E=30
export GRE2_S=220
export GRE2_E=250
export OFF_S=1
export OFF_E=30

# fuer all-ep.e
export R_KORS_P="1"
export R_LFIT="1"
export R_SHOU="1"
export R_FINAL="0"
export MAXERR_LIST="50 40 30 25 20"

# Allgemeines:
export SHIFT=0,0
export ZOFF=false } ZOFF = false -> vertical shift fixed
export ZOFF=true } ZOFF = true -> vertical shift fitted

# fuer lfit.e:
# normale Auswertung:
export RES_APP=${FILE_APP}_1
export QFLIB="xx"
export LFLIB="xx"
export TAB_APP=${RES_APP}
export KONSHIFT=1
export ICHNF=180
export ICHN=27
export ICHN_ADD=-29
export CHANNEL_A=1
export CHANNEL_B=${ICHNF}
export FACTOR_A=1.0
export FACTOR_B=1.0
export FACTOR_C=1.0
    
```



- Fit starts at that pixel (points to `export ICHN_ADD=-29`)
- Fit ends at that pixel (points to `export CHANNEL_B=${ICHNF}`)
- Weight for ErrSum in 1st region 0 < #pixel < start fit (points to `export FACTOR_A=1.0`)
- Weight for ErrSum in 2nd region start fit < #pixel < end fit (points to `export FACTOR_B=1.0`)
- Weight for ErrSum in 3rd region end fit < #pixel < end file (points to `export FACTOR_C=1.0`)

```

# nur Hot-Band;
# export RES_APP=${FILE_APP}hbs
# export LFLIB="_hb"
# export TAB_APP="_3_${RES_APP}"
# export KONSHTFT=0
# export ICHNF=120
# export ICHN=88
# export ICHN_ADD=50

# Variables for lfit.e, qflib_nls.e und lflib_nls.e (parameter for different flames):
if [ "${LFLIB}" = "xx" ]; then
export LFIT_P="4,935"
export LFIT_CONC="78,8426"
export LFIT_S_CONC="-0,00247529"
export LFIT_MIN_CONC="72,8"
export LFIT_MAX_CONC="78,1"
export LFIT_AXNRS="7,103"
export LFIT_S_AXNRS="0,000555294"
export LFIT_MIN_AXNRS="7,27"
export LFIT_MAX_AXNRS="8,45"
export LFIT_CONH2O="-0,01756235"
export LFIT_S_CONH2O="0,00005854"
export LFIT_MAX_CONH2O="0,1244"
export LFIT_CONCO2="-0,01608"
export LFIT_S_CONCO2="0,00005360"
export LFIT_MAX_CONCO2="0,1139"
fi

# fuer show*.e:
export MAXERR=25
export METHOD=29
NEW=new
APP=app

# Spreadtest:
export DT="xx"
export M1="xx"
export M2="xx"
export M3="xx"
export SPREADTEST=" ${DT} ${M1} ${M2} ${M3} "
# -----

FLAMME="FIRST-III Referenzflamme"

#
EXP_06=" 06 ${AFILE} ${DYE} 0 107 FIRST-III 41 50 ${KORSP_} ${NEW} "
EXP_07=" 07 ${AFILE} ${DYE} 0 107 FIRST-III 38 50 ${KORSP_} ${APP} "
EXP_08=" 08 ${AFILE} ${DYE} 0 95 FIRST-III 32 50 ${KORSP_} ${APP} "
EXP_09=" 09 ${AFILE} ${DYE} 0 80 FIRST-III 22 50 ${KORSP_} ${APP} "
EXP_10=" 10 ${AFILE} ${DYE} 0 62 FIRST-III 35 50 ${KORSP_} ${APP} "
EXP_11=" 11 ${AFILE} ${DYE} 0 45 FIRST-III 35 50 ${KORSP_} ${APP} "
EXP_12=" 12 ${AFILE} ${DYE} 0 37 FIRST-III 41 50 ${KORSP_} ${APP} "
EXP_13=" 13 ${AFILE} ${DYE} 0 37 FIRST-III 41 50 ${KORSP_} ${APP} "
EXP_14=" 14 ${AFILE} ${DYE} 0 30 FIRST-III 38 50 ${KORSP_} ${APP} "
EXP_15=" 15 ${AFILE} ${DYE} 0 24 FIRST-III 44 50 ${KORSP_} ${APP} "
EXP_16=" 16 ${AFILE} ${DYE} 0 18 FIRST-III 48 50 ${KORSP_} ${APP} "
EXP_17=" 17 ${AFILE} ${DYE} 0 12 FIRST-III 55 50 ${KORSP_} ${APP} "
EXP_18=" 18 ${AFILE} ${DYE} 0 3 FIRST-III 10 50 ${KORSP_} ${APP} "
EXP_19=" 19 ${AFILE} ${DYE} 0 1 FIRST-III 8 50 ${KORSP_} ${APP} "
EXP_20=" 20 ${AFILE} ${DYE} 0 80 FIRST-III 28 50 ${KORSP_} ${APP} "

# Einstellungen fuer individuelle Namelists
#   SpekNr BKG T ConN2 ConH2O ConCO2 AXNRS PRESS
# NLS_04=" 04 ${AFILE} 1600,00 54,50 0,051 0,017 8,12 0,987"

# Kommentarstrings, die via gr.e in die Ausdruecke eingebunden werde
# ACHTUNG: Keine Leerzeichen im String verwenden !!

# GR_07="TLC_1bar_Phi=2,1_r=0mm_h=5mm_Gain=90"

```

- Run **all.e** to run the fitting program. This code save all the corrected spectra (bkg, dye curve) inside **mess** folder:

- **s3a.....cor** = average of corrected single shots
- **s3s.....cor** = corrected single shots

While all the fitted spectra are saved into **lfit** folder:

- **.lft** = big file containing corrected spectrum, fit and difference (multiplied by 100) for each single shot (3 columns)
- **.sta** = table containing all the temperature fitting statistics relative to different methods; it also includes the number of spectra rejected by filters
- **.res** = results file: it contains temperature and statistics information

 Resultfile: s3s13706gd05_1.res
 11-Jul-16 16:53:36 s3s13706gd05 HTVflex0P3-FL0X FIRST-III, x=0,z=107;532:41,Dye
 :50

Method	5	6	7	20	21	26	27	29	31	32
	h/c	ch/cc	h/cc	75%	50%	6or7		LFIT	Fsum	Conc
Results	942	942	942	938	941	942	942	942	942	942
Sigma K	200	202	198	246	217	200	198	191	512	1
%	13	13	13	15	14	13	13	12	75	1
T-mean	1518	1503	1515	1606	1601	1514	1515	1570	678	75
T-mp	1449	1438	1446	1526	1540	1448	1447	1507	305	75
T-5%	1249	1240	1250	1239	1292	1247	1249	1313	160	66
(Diff.)	-200	-198	-196	-287	-248	-201	-198	-194	-145	-9
T-95%	1920	1905	1910	2049	2010	1909	1909	1952	1789	84
(Diff.)	471	467	464	523	470	461	462	445	1484	9
T-min	1022	1033	1025	967	1031	1033	1036	1126	66	73
T-max	2329	2441	2355	2604	2446	2355	2355	2372	2482	76

total Results:	filter	1	2	3	4	5	6	7	8
1200	#	46	5	0	0	0	0	0	0

maxerrsum: +2.500E+01, rejected: 207

To open the .res file it is necessary to use the **qui** program (similar to spi).

Once opened the new window, use the **open** command to read the file:

- **open [filename].res**

To see the tabled results use **show** command: it show a table with similar but more complete information than the .sta file.

Since the table is very large, filtering the results by fitting methods may simplify the visualization; to do that use **set mask** command:

- **set mask [method # method # ...]**
 e.g. set mask [20 27 29 31]

- o **_1.tab** = table showing the filtering results

```
xterm
11-Jul-2016 16:58
```

Experiment	x / mm	h / mm	Tmean / K	Sigma / K	Tmp / K	T95-Tmp / K	T5-Tmp / K	N	maxerr
13706gd05_1	0	107	1579	200	1509	472	-198	1149	.000
13706gd05_1			1576	194	1508	457	-192	1037	50.0
13706gd05_1			1574	193	1507	453	-191	1012	40.0
13706gd05_1			1572	193	1507	449	-193	977	30.0
13706gd05_1			1570	191	1507	445	-194	942	25.0
13706gd05_1			1569	191	1506	447	-194	914	20.0

```
vtmess@mc:vtmess/spray/s3a137/lfit_$
```

- o **_1_mxx.tab** = table showing the statistics about temperature measurement relative to maximum error F(Sum) = xx (it could be 0 for no filtering or 25, as default value, or any value chosen by the user)

```
vtmess@mc:vtmess/spray/s3a137/lfit_$ cat s3s137xxgd05_1_m25.tab
11-Jul-2016 16:58
```

Experiment	x / mm	h / mm	Tmean / K	Sigma / K	Tmp / K	T95-Tmp / K	T5-Tmp / K	N	maxerr
13706gd05_1	0	107	1570	191	1507	445	-194	942	25.0

```
vtmess@mc:vtmess/spray/s3a137/lfit_$
```

- o **_1_mxx_fsum.tab** = table showing the statistics about maximum error F(Sum)=xx

**** Fsum ****

Experiment	x / mm	z / mm	Fmean / 0.01	Sigma / 0.01	Fmp / 0.01	F95-Fmp / 0.01	F5-Fmp / 0.01	N	maxerr
13706gd05_1	0	107	2213	6319	305	4706	-138	1149	.000

- **_1_mxx_shift.tab** = table showing the statistics about the horizontal shift relative to maximum error $F(\text{Sum})=xx$
- **_1_mxx_ymax.tab** = table showing the statistics about the signal maximum peak relative to maximum error $F(\text{Sum})=xx$
- **.log** = log file containing all input and fitting value information


```

s3s13706gd05_1.log
File Edit Search Preferences Shell Macro Windows Help
LOG-File: s3s13706gd05_1.log
Date: 11-Jul-16 16:53:37 QUI Version: V3.4 AIX (ohne AXMD)
Spectra: s3s13706gd05.cor QFLIB: qflib137.cff LFLIB: lflib137.lib

Concentration (CONC): 78.84 %
(= CONC + S_CONC * T) (S_CONC): -.002475 %
max. allowed concentration (MAX_CONC): 78.10 %
min. allowed concentration (MIN_CONC): 72.80 %
Nonresonant background (AXNRS): 7.000 E-18 cm3/erg
(= AXNRS + S_AXNRS * T) (S_AXNRS): .000555 E-18 cm3/erg
max. allowed nonr. background (MAX_AXNRS): 8.450 E-18 cm3/erg
min. allowed nonr. background (MIN_AXNRS): 7.270 E-18 cm3/erg
Temperature (T): 300 K
Shift (SHIFT): .0000 channels
Pressure (P): 4.935 atm
No. of spectral channels (ICHNF): 180
No. of skipped spectr. channels (ICHN): 27
Channels for weighting of fsum and scaling
(CHANNEL_A): 1
(CHANNEL_B): 180
Factors for weighting of fsum
(FACTOR_A): +1.000E+00
(FACTOR_B): +1.000E+00
(FACTOR_C): +1.000E+00
Fit Offset (ZOFSET): FALSE
Accuracy (ACCREL): .1000
Max. no. of iterations (MAXF): 50
QFIT method for start temp. (QUFIT): 26
Diff. starttemp. - QFIT temp. (DIFF): .0000 K
Fitting control parameter
Temperature fitting (KONT): active
Concentration fitting (KONC): NOT active
Pressure fitting (KONP): NOT active
Spectrum shift fitting (KONSHF): active

# Time Knt Fsum T Axnrs Conc P Shift ichn QF-T Ymax
1 16:53:37 6 36.027 1753 7.973 74.50 4.935 .1663 180 1654 800
2 16:53:37 11 88.803 1409 7.782 75.36 4.935 .3494 180 1291 570
3 16:53:37 11 4.9063 1736 7.964 74.54 4.935 .3198 180 1682 3268
4 16:53:38 8 10.632 1395 7.775 75.39 4.935 .0934 180 1258 2640
5 16:53:38 8 2.5256 1706 7.947 74.62 4.935 -.0395 180 1684 17734
6 16:53:38 11 107.42 1280 7.711 75.68 4.935 .0808 180 1027 678
7 16:53:38 10 5.7453 1520 7.844 75.08 4.935 .0731 180 1405 3979
8 16:53:39 8 47.462 1412 7.784 75.35 4.935 .3139 180 1326 1100
9 16:53:39 8 8.7693 1442 7.801 75.27 4.935 -.1427 180 1301 2722
10 16:53:39 7 23.041 1570 7.872 74.96 4.935 -.0506 180 1446 1292
11 16:53:40 12 96.661 1826 8.014 74.32 4.935 -.8203 180 1847 473
12 16:53:40 12 366.47 1221 7.678 75.82 4.935 -1.657 180 915 551
13 16:53:40 7 3.2360 1592 7.894 74.90 4.935 -.2734 180 1506 11754
14 16:53:40 7 4.3463 1511 7.839 75.10 4.935 .3446 180 1451 6211
15 16:53:41 7 4.7094 1549 7.860 75.01 4.935 -.2657 180 1528 7860
16 16:53:41 7 4.4265 1481 7.823 75.18 4.935 -.2308 180 1431 13286
17 16:53:41 5 7.3452 1877 8.042 74.20 4.935 -.1674 180 1864 2433
18 16:53:41 4 9.6808 2210 8.227 73.37 4.935 .0000 180 2203 2037
19 16:53:41 7 3.4574 1352 7.751 75.50 4.935 .3320 180 1377 10839
20 16:53:41 7 2.7282 1368 7.760 75.46 4.935 -.0688 180 1350 5139
21 16:53:42 5 5.6328 1863 8.035 74.23 4.935 -.2676 180 1847 2542
22 16:53:42 8 19.233 1628 7.904 74.81 4.935 .4644 180 1486 1330
23 16:53:42 5 2.9861 1555 7.863 74.99 4.935 -.1145 180 1548 11771
24 16:53:42 7 1.6082 1417 7.787 75.34 4.935 .0499 180 1333 23504
25 16:53:42 6 19.157 1685 7.935 74.67 4.935 -.2784 180 1685 1329
26 16:53:43 12 39.296 1636 7.908 74.79 4.935 .4869 180 1510 704
27 16:53:43 6 2.4291 1800 8.000 74.39 4.935 .1759 180 1741 9626
28 16:53:43 8 16.266 1445 7.803 75.26 4.935 1.062 180 1273 1746
29 16:53:43 12 11.453 1474 7.818 75.19 4.935 -.2209 180 1340 2695
30 16:53:43 6 2.6595 1855 8.030 74.25 4.935 .2588 180 1807 5278
31 16:53:44 8 19.319 1663 7.923 74.73 4.935 .3356 180 1612 1646
32 16:53:44 6 8.2641 2181 8.211 73.44 4.935 .8663 180 2112 1040
33 16:53:44 7 8.2372 1532 7.851 75.05 4.935 .1946 180 1414 2343
34 16:53:44 7 4.0500 1636 7.908 74.79 4.935 -.2637 180 1557 9774
36 16:53:45 10 2.6364 1378 7.765 75.43 4.935 .3651 180 1285 29534
37 16:53:45 8 2.7085 1800 7.999 74.39 4.935 .6099 180 1748 9935
38 16:53:45 10 7.9013 1590 7.883 74.91 4.935 .4022 180 1561 2707
    
```

- o .dat = output of results; it also show differences in fit methods; note that the values of Fsum and Shift are multiplied by 100: this is because the code requires only integers numbers

```

s3s13706gd05_1.dat
File Edit Search Preferences Shell Macro Windows Help
Program version during data evaluation: V3.4 AIX (ohne AXMD) 15-May-13 15:35:02
Resultfile: s3s13706gd05_1.res
11-Jul-16 16:53:36 s3s13706gd05 HTVflexOP3-FL0X FIRST-III, x=0,z=107:532:41,Dye:50

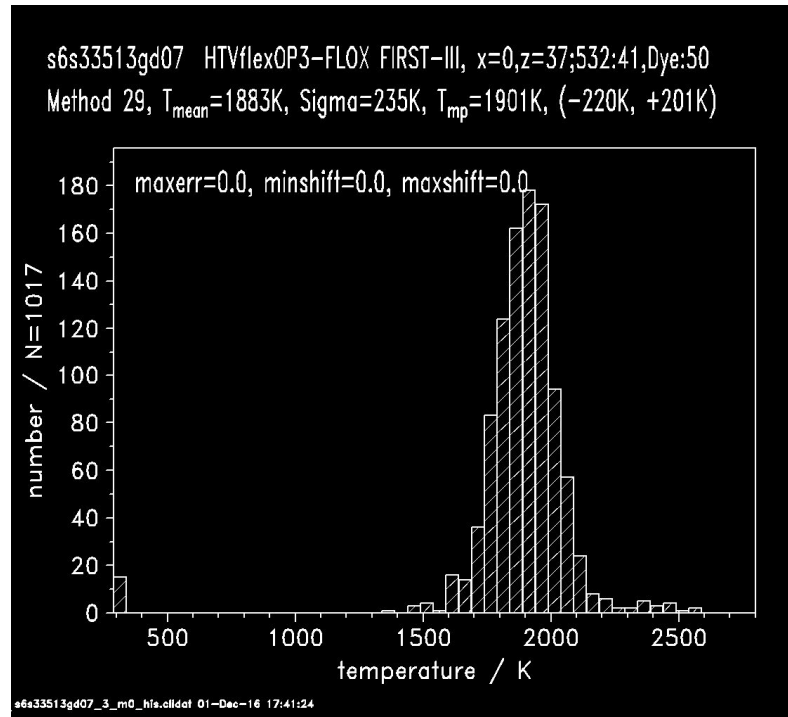
Method
# F T 6 7 20 21 26 27 29 31 33
ch/cc h/cc 75% 50% 6or7 LFIT Fsum Shift
1 0 29 1730 1654 1753 1921 1654 1654 1753 3603 17
2 0 29 1387 1291 1338 1339 1291 1291 1409 8880 35
3 0 0 1607 1682 1762 1703 1682 1682 1736 491 32
4 0 0 1339 1258 1519 1491 1258 1258 1395 1063 9
5 0 0 1634 1684 1611 1630 1684 1684 1706 253 -4
6 0 29 1240 1027 1495 1370 1027 1027 1280 10742 8
7 0 0 1504 1405 1636 1626 1405 1405 1520 575 7
8 0 29 1363 1326 1267 1526 1326 1326 1412 4746 31
9 0 0 1398 1301 1506 1484 1301 1301 1442 877 -14
10 0 0 1546 1446 1816 1698 1446 1446 1570 2304 -5
11 0 29 1965 1847 2144 1993 1847 1847 1826 9666 -82
12 0 29 1466 915 1100 1263 915 915 1221 36647 -166
13 0 0 1608 1506 1672 1738 1506 1506 1592 324 -27
14 0 0 1427 1451 1532 1600 1451 1451 1511 435 34
15 0 0 1447 1528 1561 1506 1528 1528 1549 471 -27
16 0 0 1446 1431 1435 1554 1431 1431 1481 443 -23
17 0 0 1866 1864 1676 1875 1864 1864 1877 735 -17
18 0 0 2241 2203 -1 2207 2203 2203 2210 968 0
19 0 0 1307 1377 1202 1260 1377 1377 1352 346 33
20 0 0 1348 1350 1327 1381 1350 1350 1368 273 -7
21 0 0 1935 1847 1872 2021 1847 1847 1863 563 -27
22 0 0 1601 1486 1930 1864 1486 1486 1628 1923 46
23 0 0 1461 1548 1584 1456 1548 1548 1555 299 -11
24 0 0 1396 1333 1388 1458 1333 1333 1417 161 5
25 0 0 1832 1685 1365 1854 1685 1685 1685 1916 -28
26 0 29 1571 1510 1618 1714 1510 1510 1636 3930 49
27 0 0 1761 1741 1932 1938 1741 1741 1800 243 18
28 0 0 1243 1273 1706 1556 1273 1273 1445 1627 106
29 0 0 1336 1340 1719 1512 1340 1340 1474 1145 -22
30 0 0 1779 1807 1924 1968 1807 1807 1855 266 26
31 0 0 1662 1612 1511 1817 1612 1612 1663 1932 34
32 0 0 2038 2112 2013 2285 2112 2112 2181 826 87
33 0 0 1442 1414 1598 1526 1414 1414 1532 824 19
34 0 0 1596 1557 1780 1663 1557 1557 1636 405 -26
35 1 0 0 0 0 0 0 0 0 0 0
36 0 0 1245 1285 1468 1455 1285 1285 1378 264 37
37 0 0 1737 1748 1757 1855 1748 1748 1800 271 61
38 0 0 1556 1561 1400 1600 1561 1561 1590 790 40
39 0 0 1586 1606 1718 1696 1606 1606 1659 526 35
40 0 0 1359 1268 1443 1530 1268 1268 1426 937 69
41 0 0 1446 1491 1499 1504 1491 1491 1522 213 14
42 0 0 1538 1492 1496 1623 1492 1492 1576 1570 41
43 0 0 1231 1203 1632 1416 1203 1203 1395 1498 -14
44 0 0 1343 1314 1644 1533 1314 1314 1448 950 7
45 0 0 1413 1365 1844 1612 1365 1365 1520 821 24
46 0 0 1538 1555 1338 1493 1555 1555 1541 870 10
47 0 0 1592 1511 1423 1615 1511 1511 1547 604 -32
48 0 0 1482 1467 1595 1613 1467 1467 1560 1014 34
    
```

- o `mxh_his.clidat` = histogram plot relative to maximum error F(Sum)=xx

To visualize the histogram use **charli** command:

- o **charli [filename without extension] xw**

Note that the histogram could be also obtained in ASCII format by activating **R_FINAL = '1'** in set-all.e program

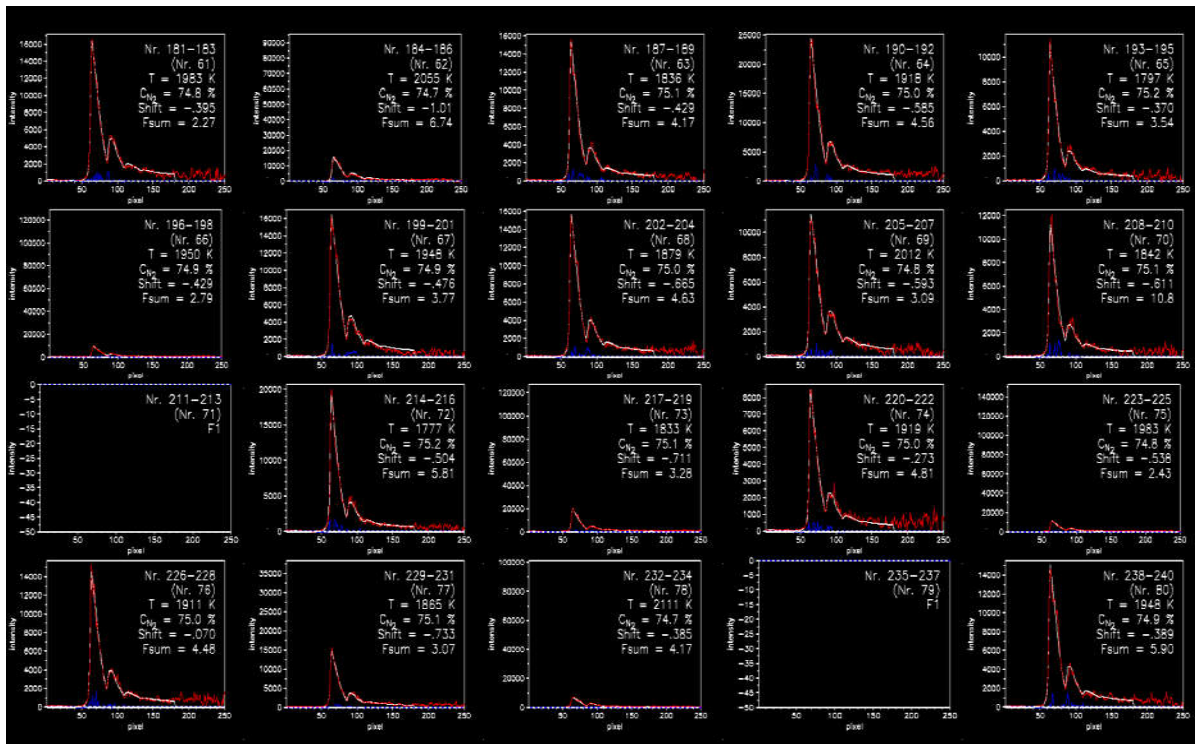


To check the quality of the fit, it is useful to use the **spl** code on **.lft** file (remember to type first **chd** and copy the filename to change the default values); then the command **@fit** display the results of the first 20 data (in principle 60 data since each single points consists in 3 columns as explained before) on the screen. To see the following data, use the command **gin -next60**. The visualization of the spectra is also useful to understand the quality of the fit and the type of filtering and the type of threshold to apply. Each plot displays the temperature value and some information about the rejection of the data point from the statistical analysis:

- **F1** = filtered for too low counts (close to background level)
- **F2** = filtered for too high counts (camera saturation)
- **T** = Threshold for a too high F(Sum) (bad fit)

As alternative you can use the **show-fit.e** command:

- **show-fit.e [name of file] [xmin] [ymin] [ymax] optional)**



Based on these numbers, the **.tab** file and the visualization of the fit it is possible to evaluate the quality of the spectra and eventually change the threshold parameters (rarely the fitting method) to obtain better results. Iteration on the used parameters may occur.

Usually one of the reasons of a bad fit is a bad horizontal shift; the code is not good in fitting temperature and shift at the same time, so providing the exact shift (± 1 pixel) will improve a lot the fit and decrease the F(Sum) value. To change the starting position it is necessary to edit **ICHN** value in **set_all.e** program inside **mess** folder.

Sometimes the criteria to exclude one spectrum from the fitting (because the signal is too low or the signal saturates the camera) are not well set for the experiment. To modify these criteria, edit **lfit.e**:

- **set filter** = how many and which type of filters are in use
- **set fparam 1** = filtered for too low counts (250 default value)
- **set fparam 2** = filtered for too high counts - saturation (64000 default value): this filter takes into account also the bkg subtraction and the dye curve correction: so, this value could be lower than the "nominal" 65000 counts for camera saturation.

```

lfit.e
File Edit Search Preferences Shell Macro Windows Help
date +%e-%b-%Y %H:%M" >${LOGFILE}
#
if [ ! "$ZOFFSET" = "false" -a ! "$ZOFFSET" = "true" ]; then
  echo "wrong option for 'set lfit -zoffset ...'"
  exit
fi
#
# alles zwischen "<<eof" und der Zeile "eof" wird zu QUI geschickt!!!!!!
# falls ein '$'-Zeichen zu QUI geschickt werden muss, muss ein '$'
# geschickt werden. '$' wird von AIX interpretiert, da "<<eof" gesetzt ist!!
#
# *****
cd ${DIRLFIT}
qui batch <<eof >>${LOGFILE}
set break warning
|-----
set method 1 2 3 4 5 6 7 9 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 29 31
set filter 1 2
set fparm 1 250
set fparm 2 64000
|-----
set lfit -p ${LFIT_P}
set lfit -conc ${LFIT_CONC} -s_conc ${LFIT_S_CONC} -max_conc ${LFIT_MAX_CONC} -
set lfit -axnrs ${LFIT_AXNRS} -s_axnrs ${LFIT_S_AXNRS} -min_axnrs ${LFIT_MIN_AX
IPol, CARS:
|set lfit -axnrs 0,0 -s_axnrs 0,0 -min_axnrs 0,0 -max_axnrs 13,0
set lfit -kont 1 -konshf ${KONSHIFT} -konc 0 -quickfit 26 -accrel 0,1
# set lfit -konc 1 -conc 75,0 -s_conc 0 -max_conc 200 -min_conc 0
set lfit -zof ${ZOFFSET}
set lfit -shift ${SHIFT_START}
set lfit -channel_a ${CHANNEL_A} -channel_b ${CHANNEL_B}
set lfit -factor_a ${FACTOR_A} -factor_b ${FACTOR_B} -factor_c ${FACTOR_C}
|-----
set lfit -ichnf ${ICHNF}
chc ${OFFFILE}
lfit ${LFFILE} -analyze -all
set comb 6 7 -ramp
|-----
RD_DATE ${FILE} ${RD1}${RD2};${RD3}
!!!!!! open ${RESFILE} -cre
open ${RESFILE} ${RESFILE_CREATE}
sho -filter

```

Note that it is possible to convert each single column of data from .lft file to ASCII file; this could be useful to export some spectra on Windows machine and plot them. However, this procedure can convert and save only one column per time.

Use spi program and open the .lft file as explained above.

Then use the command:

- o **load -mmf x** where x is the column # (remember: for each measurement point there are 3 cols: data, fit and difference * 100)
- o **save name.ascii - asc** saves the selected column as ASCII with the chosen name

It is also possible to fit the average of the spectra instead of the individual single shots. In lfit.e replace the "s" in the base filename with an "a".

```

RD1="HTVf1exOP3-FLOX "${6}", "
RD3="532:${RD4},Dye:${RD5}"
# -----
FILE=${PRE}s${TAG}${NUM}${AFILE}          Replace with an "a" to fit average spectra
EXPFIL=${DIRMESS}${FILE}.cor
QFFILE=${DIRQFLIB}qflib${TAG}${QFLIB_}
LFFILE=${DIRLFLIB}lflib${TAG}${LFLIB_}.lib
RESFILE=${PRE}s${TAG}${NUM}${RESAPP}
LOGFILE=${DIRLFIT}log/`basename $0 .e`_${NUM}${RESAPP}.log
if [ ! -d ${DIRLFIT}/log ] ; then mkdir ${DIRLFIT}/log ; fi
date +"%e-%b-%Y %H:%M" >${LOGFILE}
# -----
if [ ! "$ZOFFSET" = "false" -a ! "$ZOFFSET" = "true" ] ; then
  echo "wrong option for 'set lfit -zoffset ...'"
  exit
fi
# -----

```

Finally create and save the final results (final table and histograms) in ASCII file, readable on Windows machine. Modify **showfinal.e** in **lfit** folder:

- **AFILE** = last part of the basenamfile
- **MAXERR** = filter for maximum err(Sum)

Remember to list all the run # in the experiment at the end of the program otherwise the code stops at the last #.

```

showfinal.e
File Edit Search Preferences Shell Macro Windows Help
# show.e 5-Aug-98
# Display statistic of result file
# 25-Oct-99 also with speadtest
# load variable definitions:
# ../mess/set.e
-----
cd ${DIRLFIT}
NUM=00
-----
#
if test $# -ge 6 ; then
  NUM=${1}
  if [ ! "${2}" = "xx" ]
  then
    AFILE=${2}
  else
    AFILE=""
  fi
  XVAL=${4}
  YVAL=${5}
  MAXERR1=${7}
  MAXERR2=${8}
  MAXERR3=${9}
  MAXERR4=${10}
  MAXERR5=${11}
  NAME=${12}
  TEST_T=${13}
  TESTM1=${14}
  TESTM2=${15}
  TESTM3=${16}
else
  echo "use: $0 <number> <add to filename> <<x-Ort> <y-Ort> <z-Ort> "
  echo "      <maxerr1> <maxerr2> <maxerr3> <maxerr4> <maxerr5> "
  echo "      <name of tab file> <delta-T> <test M1> <test M2> <test M3>"
  exit
fi
-----
#
MAXSHIFT="0.0"
MINSHIFT="0.0"
AFILE="Fd39_1"
if [ "${NUM}" = "04" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "05" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "06" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "07" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "08" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "09" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "10" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "11" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "12" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "13" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "14" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "15" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "16" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "17" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "18" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "19" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "20" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "21" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "22" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "23" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "24" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "25" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi
if [ "${NUM}" = "26" ] ; then MAXERR="40" ; TEST_T="300" ; TESTM1="26" ; TESTM2="29" ; fi

```

Other filtering options are available: check the user manual or contact Dr. Lückerath for further details. One option is to filter unbalanced cold and hot part of Nitrogen spectrum once the measurement was performed in a region where hot and cold spectra are simultaneously present: in this case the fit would be very poor even if the err(Sum) is low. The filter check the difference in temperature between two different methods and discard the measurement if the discrepancy is above an imposed threshold.

- **TEST_T** = maximum temperature difference
- **TESTM1** = # of method to compare with (usually use 26 which is the combination of method 6 – cold hot/cold cold – and method 7 – hot / cold cold-)
- **TESTM2** = fitting method (default 29)

Then go to **mess** folder and enable in **set.e** only **R_FINAL="1"** (set to "0" all the other R_ parameters). Enable all the run # you want to process in **all.e** and run all.e for the last time.

The final table and histograms are created in **lfit** folder; however the table is not designed for an easy import in excel (or origin), so to remove the table borders, run **replace_tab.e**:

- **replace_tab.e [tab name without extension]**

Sometimes check the status of the MC machine memory since the storage is limited. To do so use the **dfu** command directly in any folder. If the memory is full, create a compressed backup file (.tar) in data1 partition:

- **tar -cvf /data1/cv/vtmess/[name of the file].tar [name of the folder]**

Once the tar file is completed, copy it on Windows through a FTP program as backup file and free both data1 and data2 memory.

8. Print results

It is possible to print directly from the MC machine:

- **export RZ_POST = vt-p-05**
- **echo \$RZ_POST**

or from charli:

- charli xw
- charli z2su

print on screen

print on printer

or from gino:

- gino -noopt -pform z2su -nodash
- gino -opt -pform xw
- gino -ps

print on printer

back to screen

alternative method for printer