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Proposal for a new parameterisation of the instrumental spectral response function in DOAS retrievals and application to satellite measurements

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The instrumental spectral response function (ISRF) is a key quantity in spectroscopy. Within DOAS retrievals, the ISRF is needed for an accurate wavelength calibration and for the convolution of trace gas cross-sections to instrumental resolution. DOAS analysis software like QDOAS or DOASIS allow the fitting of a high resolution solar spectrum to a measured spectrum based on a parameterized ISRF with predefined shape (e.g. Gauss, Lorentz, Voigt). For OMI, a more advanced ISRF ("broadened Gauss") was determined which allows for flat-top and asymmetric ISRF; however, this ISRF model is computationally expensive due to the high number of parameters.

Here we propose a “Super Gaussian” as further model function for the ISRF, which is similar to a Gaussian, but with the exponent ξ as additional free parameter:

$F(x) = A * exp(-(|x|/w)^{\xi})$

The parameter w determines the width of F, while ξ basically determines the shape. Optionally, different values for ξ and w can be allowed for the left vs. right branch of F to construct asymmetric ISRFs.

This model function was found to be a good compromise between good fit results (i.e., F represents the actual ISRF much better than a Gaussian) for a wide range of tested ISRF shapes on the one hand, and robustness of the fit and low computation time on the other hand due to the low number of free parameters.

A further advantage of this description of the ISRF is that the two partial derivatives, representing changes of shape and width, respectively, allow to mimic potential spectral structures caused by temporal changes of the ISRF (e.g. due to changes of the detector temperature) by adding pseudo-absorbers in the DOAS analysis. We investigate how far this affects different trace gas retrievals from satellite measurements.