TIDE: Distributed end-to-end simulation of an Earth Observation system effectively supports design-to-cost trade-offs

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INTRODUCTION

TIDE is a tool to support the design process for remote sensing instruments and was in particular developed for the TROPOMI on ESA's Sentinel 5 Precursor satellite. It provides an environment to compute products and error budgets for different design options as input for design trade-offs.

The strong points for TIDE are the following.

- TIDE products and error budgets are on Level 2 data products, making it an End-to-end tool

- It uses realistic input scenes for input, from e.g. atmospheric chemistry transport models

- It is grid-based, and uses the grid to perform parallel processing of the various scene ground pixels of the scene

TIDE consist of a generic grid tool (GridAssist) and a part specific to atmospheric remote sensing. This is tuned for TROPOMI but would be directly applicable for other UV-SWIR sun backscatter instruments. For other types of instrument more significant adjustments would be necessary.

The tool is anyhow meant to be used throughout the complete instrument development cycle, from early phase zero up to in-orbit check-out in phase E. This is possible because it consists of a chain of modules which can be made to contain increasing complexity towards the later phases.

The remote sensing modules are from different partners with a special property that all parties can access all modules, including those from other partners, but the owners are the ones that provide the module and documentation. Thereby they control the information given and are able to preserve property rights. This is an important novel quality as it allows all partners to use the TIDE for their own roles within the project, without requiring an additional effort from the other partners The TIDE has the following advantages:

- Reduced risk of over-design: instrument designers can design an instrument based on level 2 output, rather than on the intermediate level 1b. This reduces the number of actions for the science partners and hence increases efficiency.

- The science partners can easily use realistic scenes for test and specifications. This will increase the understanding of the possibilities (and hence the limitations) of the instrument design.

- The end user partner can easily familiarize himself with the intricacies of the level 2 data concerning its contents and its format. In the past complexity of the data products and underlying intricacies lead to a situation where the products were difficult to handle. Early access of the end user to these products increases the overall efficiency.

The partners in TIDE are Dutch Space (lead, grid system, scene generator, instrument simulator, 01b processor and error analyzer), KNMI (UV-NIR radiative transfer model and NO_2 retrieval), SRON (SWIR radiative transfer model and CO/CH_4 retrieval), BMT ARGOSS (scene generation and commercial user aspects) and TNO (parameters for the instrument simulator).

The TIDE was first presented to ESA during the Concurrent Engineering for Space Applications Workshop (Oct 2006, it was called IDEE then [1]) where it was considered as an important development that allows a way of concurrent engineering throughout all development stages of a project. Considering the generality of the setup of the TIDE, we consider it to be applicable to instrument development projects other than TROPOMI.

TROPOMI INSTRUMENT

TROPOMI will perform global measurements of trace gases in the troposphere and stratosphere and is planned to be launched in 2014 on ESA's Sentinel-5 Precursor satellite. After the successful missions of SCIAMACHY (launched 2002 on ENVISAT) and OMI (launched 2004 on NASA's AURA satellite), TROPOMI is the follow-up instrument combining and increasing the capabilities of SCIAMACHY and OMI. SCIAMACHY [2] is a scanning spectrograph covering the wavelength range between 250 and 2400 nm, with a nadir ground pixel size of 30x60 km^2 and a global coverage in 6 days. OMI [3] spans the wavelength range between 270 and 500 nm, but covers the Earth in a single day, with a nadir ground pixel size of 13 x 24 km^2.

TROPOMI will cover the full wavelength range between 270 nm and 500 nm, plus a near-IR band at 675-780 nm and a SWIR band at 2305-2385 nm [4][5]. Its ground pixel size is improved to 7 x 7 km^2. TROPOMI covers the complete globe again in one day and it has much better sensitivity compared to OMI and SCIAMACHY.

The products retrieved from the various channels are the following.

- UV1 Ozone vertical distribution

- UV2: SO2, O3, HCHO, BrO, OClO, aerosols

- VIS: NO2 and aerosols

- NIR: cloud top height, H2O, aerosols
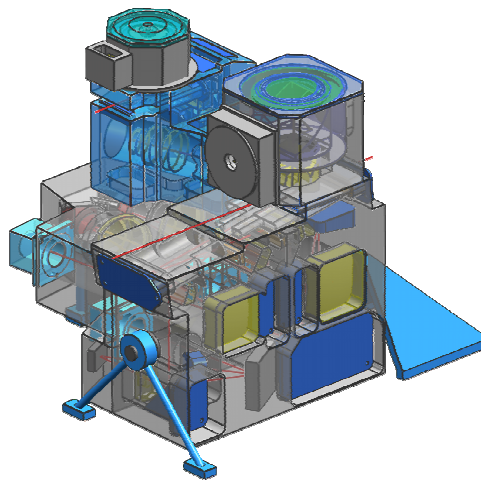
- SWIR: CO and CH4

Fig. 1   TROPOMI instrument

TIDE's ATMOSPHERIC REMOTE SENSING TOOL

The TIDE tool consists of two main parts, the general grid processing tool 'GridAssist' and the series of modules forming the atmospheric remote sensing tool. These modules are executable tasks that deal with observed scenes and atmospheric and instrumental details. This section describes the atmospheric remote sensing tool and the next section is devoted to the more general GridAssist tool.

The TIDE is a computing chain consisting of the following modules:

- Scene generator
- Radiative transfer models for UV-NIR and SWIR
- Instrument simulator
- Level 01b processor
- Level 1-2 product retrieval algorithms for firstly NO2, CH4 and CO
- Error analyzer

The modules have the following functionality:

- The Scene Generator firstly defines the scene in terms of trace gas constituents, albedo and atmospheric conditions. Secondly, it defines the satellite flight and instrument viewing. Lastly, it also defines the settings for instrument simulator and level 0-1b to have the overview of the simulation centered at the Scene Generator.
- The Exposure Generator is a simple tool to separate the various exposures contained in the Scene.
- The Radiative Transfer Model (RTM) takes viewing and sun angles and all atmospheric and albedo parameters to generate radiance spectra for every viewing pixel from the Scene.
- The Instrument Simulator takes the radiance spectra in the swath of a single exposure and generates the raw instrument response.
- The Level 0-1b Processor takes a Level 0 product and converts this to calibrated radiances, the level 1b product.
- The level 1-2 Processor computes the trace gas products from the Level 1b product.
- The Error Analyzer compares products directly delivered from the input Scene and the Level 2 products. The results are written in an Error Matrix for each of the products.

These modules are basically executed as a sequence, as shown in the flow diagram in fig. 2. The modules within the loop over the exposures in the flow diagram are automatically processed in parallel by the grid.

We use the Dutch Space GridAssist toolset that takes care of all workflow and access handling management and provides the distributed environment to allow all partners to access the TIDE. It also provides the modules as executable tasks, thereby safeguarding the proprietary aspects of the software for all partners separately.

Especially the Instrument Simulator and its inverse, the Level 01b processor, are set up in a way that allows the complexity to grow during the total development period of the TROPOMI. For this purpose, the simulator is almost fully configurable and allows switching between simple instrument descriptions, full modeling detail just before instrument finalization and including measured characterization data just before final delivery.
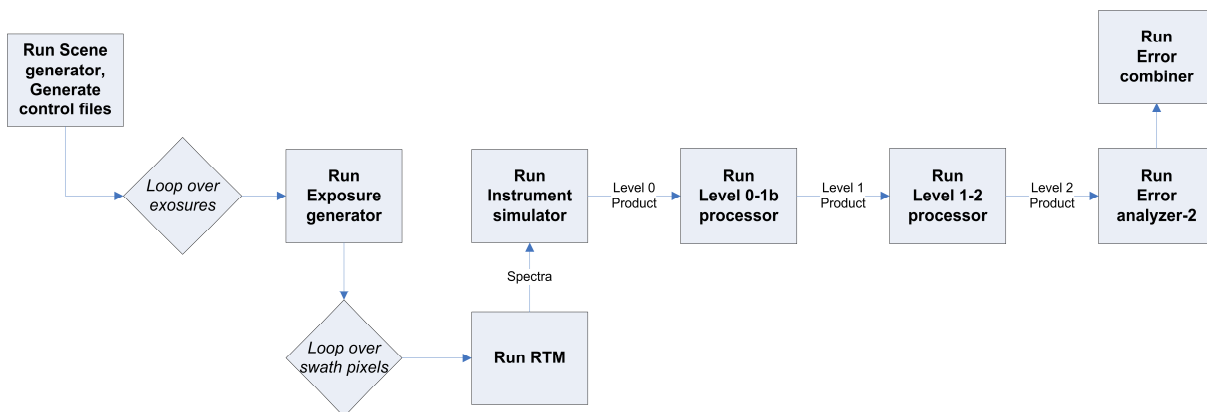

Fig.2   Flow diagram with the TIDE remote sensing applications

GRID PROCESSING AND GRID ASSIST

Having defined the components from the 'Atmospheric Remote Sensing tool',
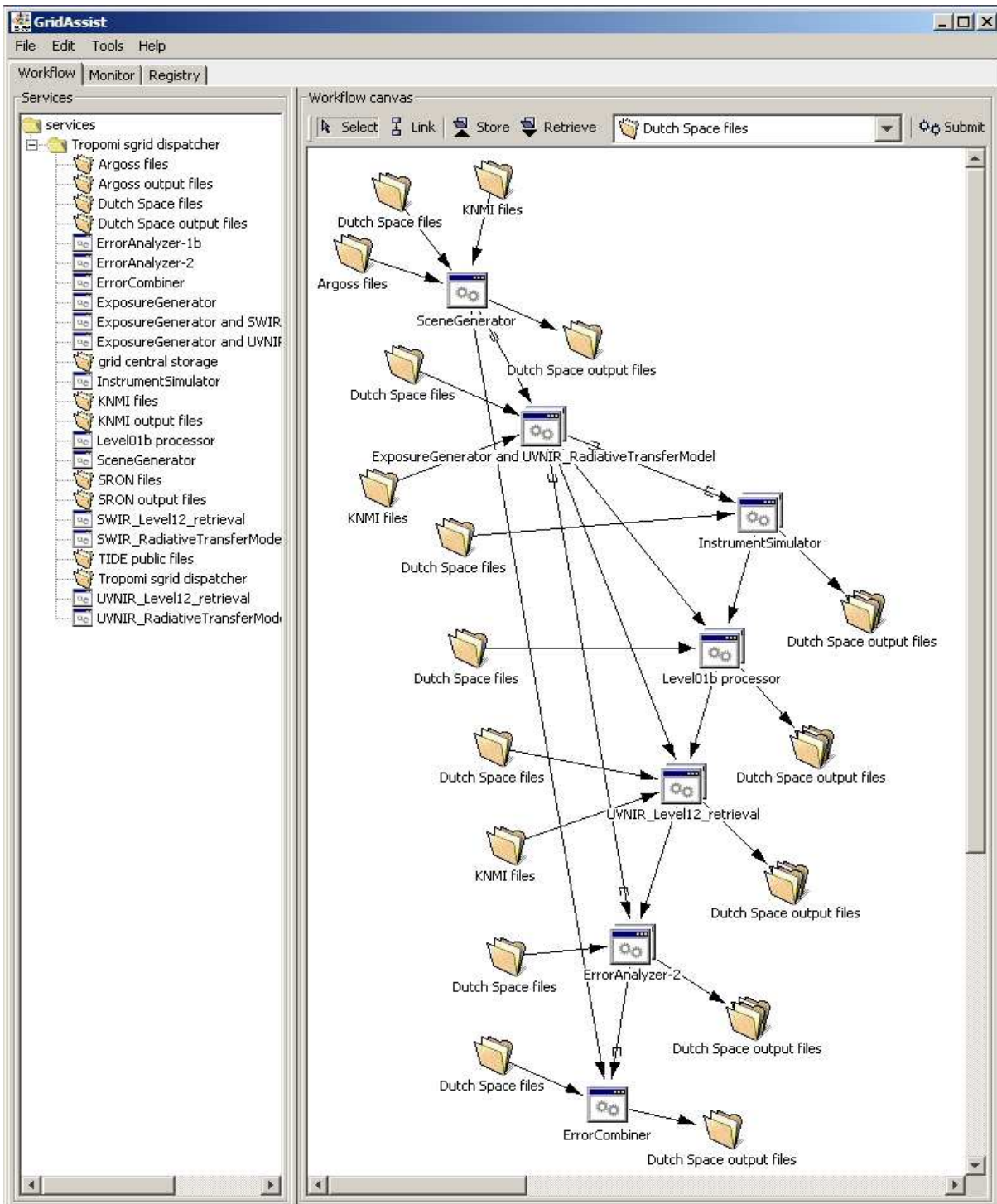This section describes the GridAssist tool.

Fig.3 GridAssist implementation of the processing flow from Fig. 2

The TIDE makes use of the GridAssist software framework, which in turn utilizes the Grid computing system. GridAssist is developed and maintained by Dutch Space. Grid computing is a form of distributed computing where a virtual computer is created, which consists of a cluster of networked computers that act together to perform large computing tasks. The clustering of the network is usually fairly loose. GridAssist is a software framework that provides benefits of computing in a Grid environment to applications that are not inherently 'Grid-aware', for users who are not experts on Grid technology. It provides a portal for access to applications, resources and data using high-speed networks, a scenario builder and a controller for scheduling jobs.

A key component of GridAssist is its graphical user interface. Hidden behind the GUI is a lot of complex technology that the user need not be aware of. An example of the GUI created by GridAssist is shown in fig. 3.

The left palette shows three tabs:

- Workflow:
  The GridAssist Workflow Pane allows the user to construct workflows in an easy way. The tool provides a graphical user interface where the user can create workflows using the drag-and-drop principle.

- Monitor:
  The GridAssist Monitoring Pane allows the user to track the progress of the jobs that he/she created in the GridAssist Workflow Pane. It also allows the user to terminate a job.

- Registry:
  The GridAssist Registry Pane can be used by administrators and application integrators to manage the information about applications and resources available for the user. This information is stored in the GridAssist Registry.

The large window on the right contains the main graphical display of the workflow. Three main items can be used:

- Applications:
  Applications are the executable programs.

- Data Storage:
  These are the directories where the input and output data are stored. The files that are transferred can be viewed by moving the mouse over the connection that links to the Data Storage.

- Data connections:
  Between applications themselves and between applications and data storage, data connections need to be established. The workflow tool will check the correctness of the connections between the services, by checking that the output produced by one application matches the type of input required or expected by the destination application.

The GridAssist workflow tool greatly assists in easily setting up a workflow. Here we describe the main steps that need taken to build such a workflow.

First the user starts the Workflow Tool on his local client machine where GridAssist only needs Java RE to run. The next step is that the tool queries the Registry in order to obtain information about available services. The workflow tool presents these services in a kind of palette in the left panel. The items in that left panel can now be dragged-and-dropped in the right panel. In the right panel, they will appear as icons.

Now, the most important step is to connect the selected services. This is done by first clicking on the "link" button at the top of the right panel and then by drawing a line between the two services. The contents of the connection can be inspected by moving the mouse over the line (e.g. the file to be written is shown), and edited by double clicking on the line. When the user has completed defining the workflow, it can be saved as a local file for later use. The next step is to click the submit button, which submits the workflow to the Workflow Controller. After the workflow has been submitted, it will be processed automatically, without requiring user intervention.

TIDE IN USE

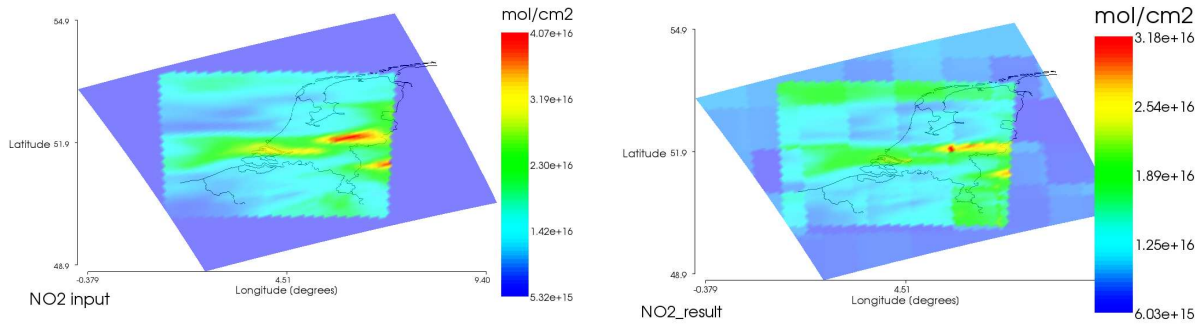In this section we show some analyzes results with NO_2 in the Netherlands.

Fig. 4 NO2 input scene (left graph) and TIDE result (right graph) revealing underlying effects (1 degree resolution albedo map) and incomplete air mass correction for the NO_2 algorithm

Fig. 4 shows on the left a scene above the Netherlands and on the right the TIDE result from this scene. The result is not exactly equal to the input, because TIDE does not adjust the vertical profile of the NO_2 and meteorological conditions as is done in the operational processing. The effect is that the main structure is correct, the absolute NO2 values have some error and the image shows a residual from the underlying albedo map. This albedo is a wavelength dependent 1°x 1° map and the result shows the 1°x 1° structure. The result in Fig. 4 does not include instrument noise and digitization and Fig. 5 shows a result including the instrument noise and also the underlying albedo map.
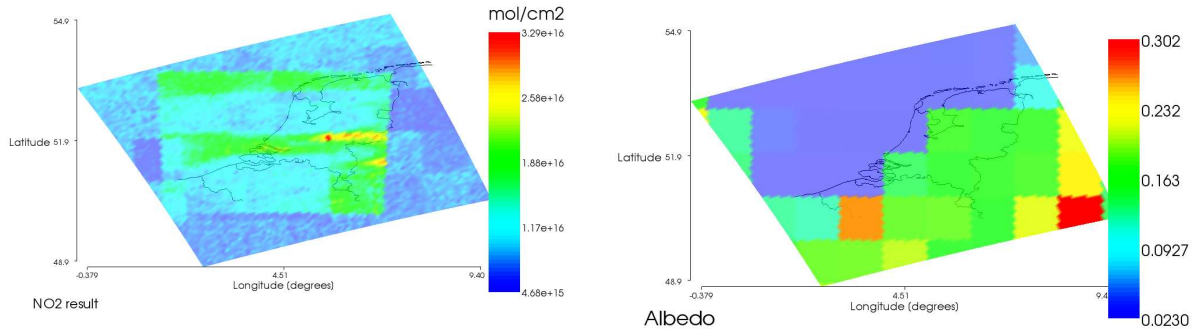

Fig. 5 NO2 TIDE result including instrument noise and digitization effects (left graph) and the underlying albedo map for a visible wavelength (right graph)

To extract the effect from the instrument digitization separately, we compute an error from the Fig. 5 result and using right graph in Fig. 4 as reference, as follows.

$$\varepsilon_{i,j} = \frac{NO2_{i,j} - NO2ref_{i,j}}{NO2ref_{i,j}}$$

Where
$\varepsilon_{i,j}$ relative NO2 error for pixel i,j
$NO2_{i,j}$ NO2 result (Fig.5 graph)
$NO2ref_{i,j}$ NO2 reference result (Fig.4 graph)

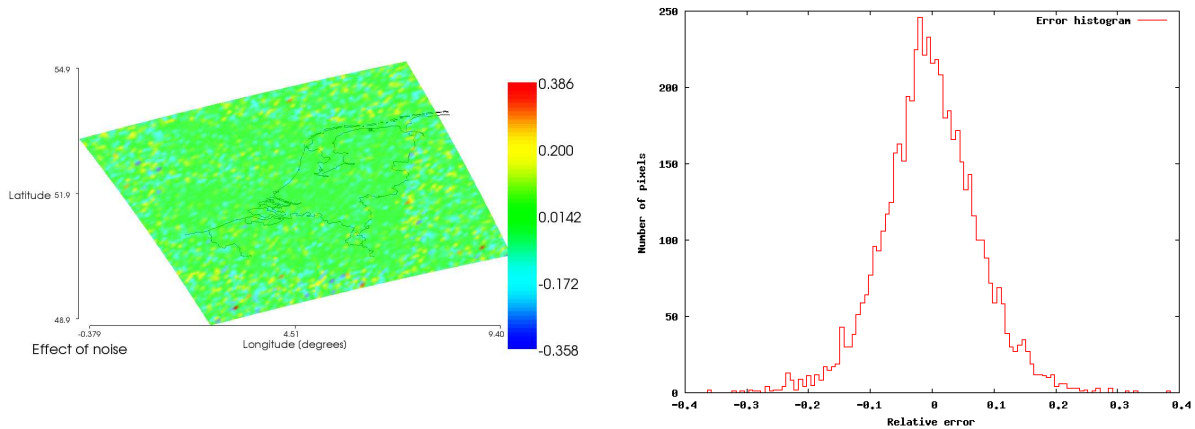The relative error computed in this way allows easy evaluation as shown in Fig. 6.

Fig. 6   NO$_2$ relative error result shown as geo-located image (left graph) and shown as histogram distribution (right graph)

As engineering example we add the effect from a mis-alignment error in the VIS detector. Errors in this alignment mean that different wavelengths from the same spectrum do no observe exactly the same ground pixel meaning that we have a co-registration error.

The effect is introduced by distorting the wavelength and viewing matrices in the instrument simulator. This distortion can be done in a number of ways, by shifting, rotating, sine or polynomial distortion or by introducing a matrix with pixel locations from optical design ray tracing models.

Fig. 6 shows NO$_2$ results after rotating the VIS detector by 0.06 and 0.5 degrees. It should be clear that an error of 0.5 degrees should be unacceptable but even 0.06 degrees has impact on the product.
These results can be used to set up hardware alignment and stability budgets and/or to optimize the Level 1-2 algorithms to be least sensitive to the errors once they are known.
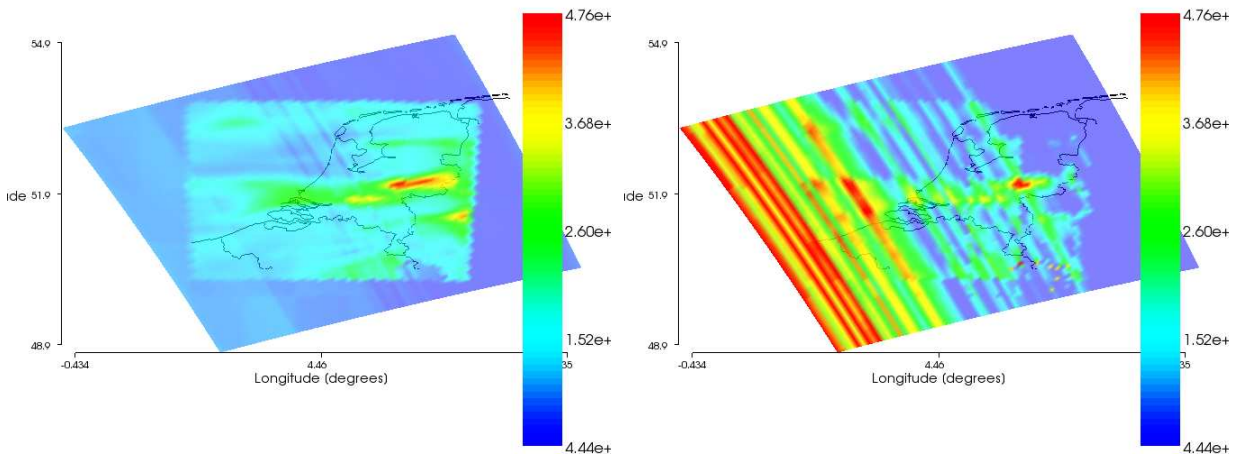

Fig. 7   NO$_2$ results including a co-registration error in the instrument simulator (left graph 0.06 and right 0.5 degrees)

CONCLUSION AND OUTLOOK

The TIDE tool is very powerful, firstly to support TROPOMI development and potentially for other instrument missions as well.

As it allows rapid evaluation of the impact of instrument design parameters on the science data products of the mission it is indispensible for doing design trade-offs in the early phases of the project. The tool is in use now to analyze the specifications of a simplified TROPOMI definition resulting from a recent cost drive.

To reap full benefit of the tool, there are aspects which will still need some development.

Firstly, for the science partners TIDE allows to test the Level 1-2 product algorithms for realistic scenes and detailed instrument properties. This is a potential which requires these partners to upload up to date versions of their algorithms to the TIDE environment and also to have their algorithms in a form that meet the interface requirements towards the other modules and it requires the Scene generator to control the latest algorithm versions. These aspects are complex and take some time before they are common practice.
A maybe more serious issue is the necessary limitations in the radiative transfer models in the sense that these RTMs for full cloud and aerosol models may require several hours of processing to obtain a single radiance spectrum. This is, even in a grid system, not very practical and therefore TIDE runs normally exclude aerosols and have very simple cloud models. This at present somewhat limits the use.

For the instrument developers TIDE provides a very important benefit in the sense that it allows to check the imposed Level 0 or Level 1b instrument requirements in the context of complete scenes. As such, it allows discrimination of rare and common cases and on the whole it allows evaluation of the requirements. This allows the instrument developers to find cost drivers and discuss these on the basis of end-to-end performance with the scientists and project customers such as e.g. governments or ESA. This is clearly a new role for the instrument developer and for the customer. However, the complexity of current and future instrument projects is significant and we expect that the new opportunities created with TIDE will find its way, both useful for the developer and the customer.

We expect to continue using the TIDE for the TROPOMI development.

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