

Description of the new diagnostic, Integrated Reaction Rates (IRR)

The MOZART chemistry options (chem_opt = 112, 201, 203) can now be run with a new diagnostic that outputs the time integrated gas-phase reaction rates (IRR) of the chemical mechanism. This capability is similar to the integrated reaction rate analysis in the Community Multiscale Air Quality Modeling System (CMAQ).

The namelist.input file has added options to run with this diagnostic and there is a new input file, wrfchem_irr_diag_d<domain>, that needs to be in the simulation run directory.

In namelist.input, the following must be included in order to get the IRR output files.

In the &time_control section, the following must be added:

```
auxhist9_outname      = "IRR_DIAG_d<domain>_<date>"
auxhist9_interval_h  = 1,1
frames_per_auxhist9  = 1,1
io_form_auxhist9     = 2
```

In the &chem section the IRR option must be added:

```
irr_opt = 1
```

The variable irr_opt is set on a per-domain basis.

The wrfchem_irr_diag_d<domain> file is a text file containing a list of reactions, one per line, that will be output to the IRR output file. If the user would like all the gas-phase reaction rates in the output file, then one simply puts "all" in the wrfchem_irr_diag_d<domain> file. As an example, to put the following 3 integrated reaction rates in the IRR file, the wrfchem_irr_diag_d<domain> file contains:

```
NO2+HV
NO+O3
O+M
```

To put 3 integrated reaction rates in the IRR file, the wrfinput_irr_d<domain> file contains:

```
All
```

As the file name indicates, wrfchem_irr_diag_d<domain> is for a specific domain of the model run.

The IRR output files are named IRR_DIAG_d<domain>_yyyy-mm-dd_hh:mm:ss. The files are netcdf files containing 4-dimensional arrays for each IRR. For example, for NO2 + HV the output array name is NO2_HV_IRR. If two reactions have the same two reactants (e.g. O3 + HV), then there will be an "a" associated with the second reaction's output name, O3_HV_a_IRR. These 4-d arrays contain output for each grid point in the model domain, and are the time integral of

the reaction rate starting from the simulation initial time to the time of the output. Thus subtracting the 11:00:00 output from the 12:00:00 output yields the change in the integrated reaction rates over the hour from 11:00:00 to 12:00:00. See the README.irr_diag file in the top level WRF directory for more details.

The output can be used with the Process Analysis tool, PERMM (Vizueté et al., xxxx). At this stage, we do not yet have python scripts in place to share with the community. If you plan to use PERMM with the MOZART chemistry and require advice with the analysis of the output, then please contact us.

PERMM is setup for both IRR and integrated physical rates (IPR). The IPR has not been added to WRF-Chem, but the same information can be output in the wrfout file via other diagnostics. In particular, the chem_diag option (see WRF-Chem User's Guide for more information) will output vertical and horizontal advection tendencies, vertical mixing (including dry deposition), convective transport, and the total chemistry tendency. The emissions of specific compounds can be placed in the wrfout file by adding them to the io_fields file. For example, anthropogenic emissions of NO are found from the E_NO variable. Biogenic emissions of, e.g. isoprene, are in EBIO_ISO if using the MEGAN biogenics emissions parameterization. Fire emissions of NO are in EBU_NO. All the fields are defined in the registry.chem.