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Supplement of

A new Lagrangian in-time particle simulation module (Itpas v1) for atmospheric particle dispersion

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S1 Additional Figures

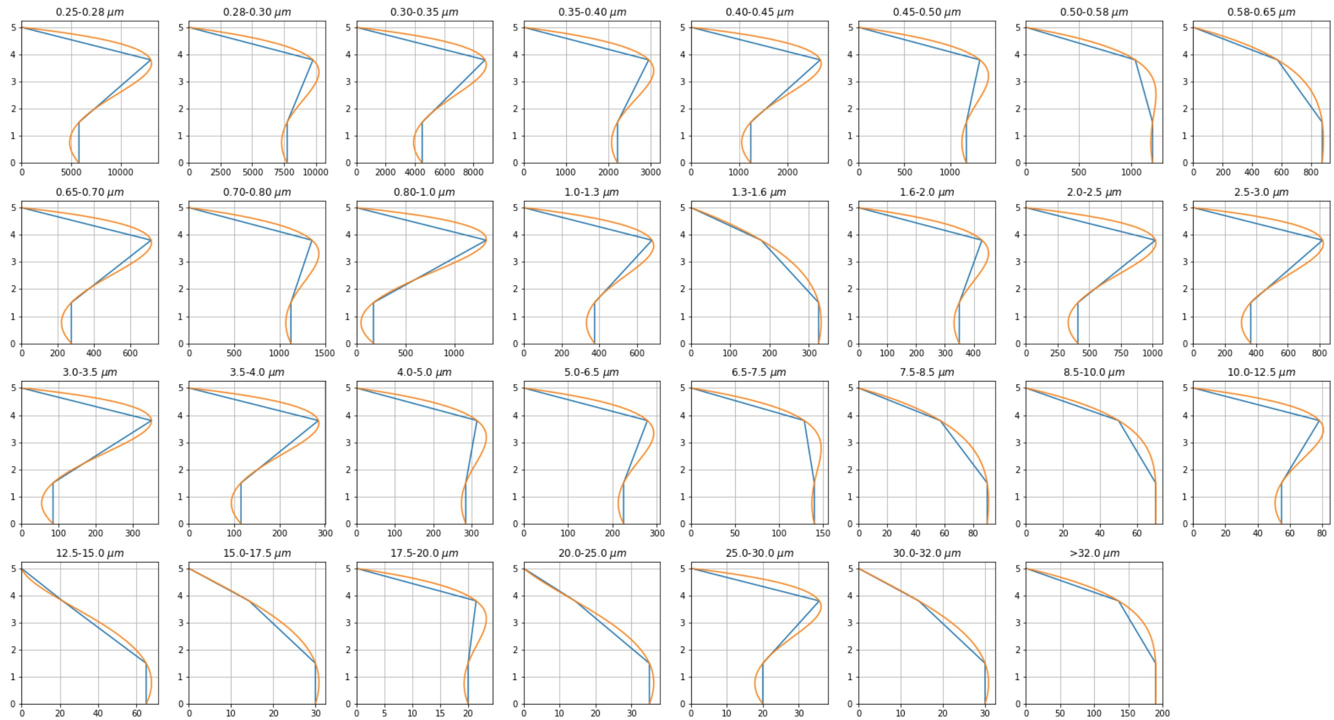

Figure S1. EXP1: Vertical profiles of the particle concentration [particle per litre] for each size bin of the Environmental Dust Monitors; Blue: Measurement; Orange: Polynomial fit; Please note that the scaling of the abscissas vary

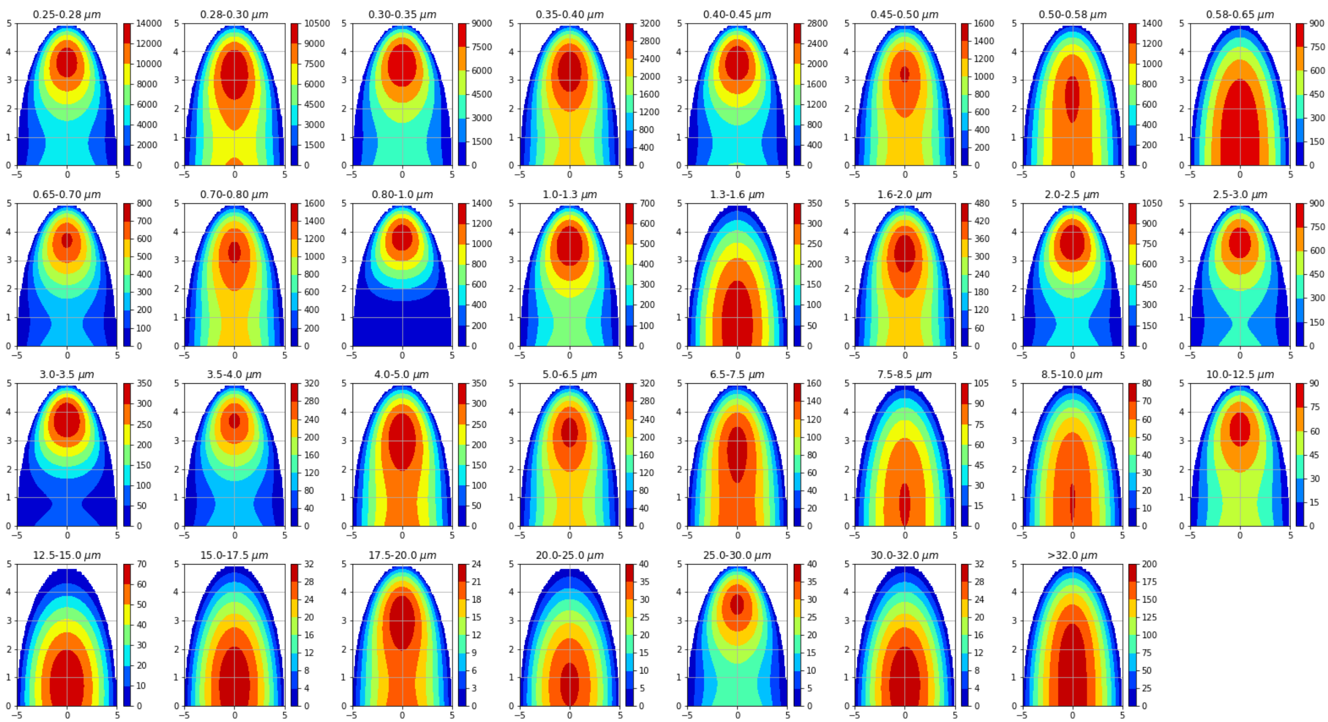

Figure S2. EXP1: Cross-section through the initial particle concentration field [particle per litre] for each size bin of the Environmental Dust Monitors; Please note that the scaling of the colour bar vary

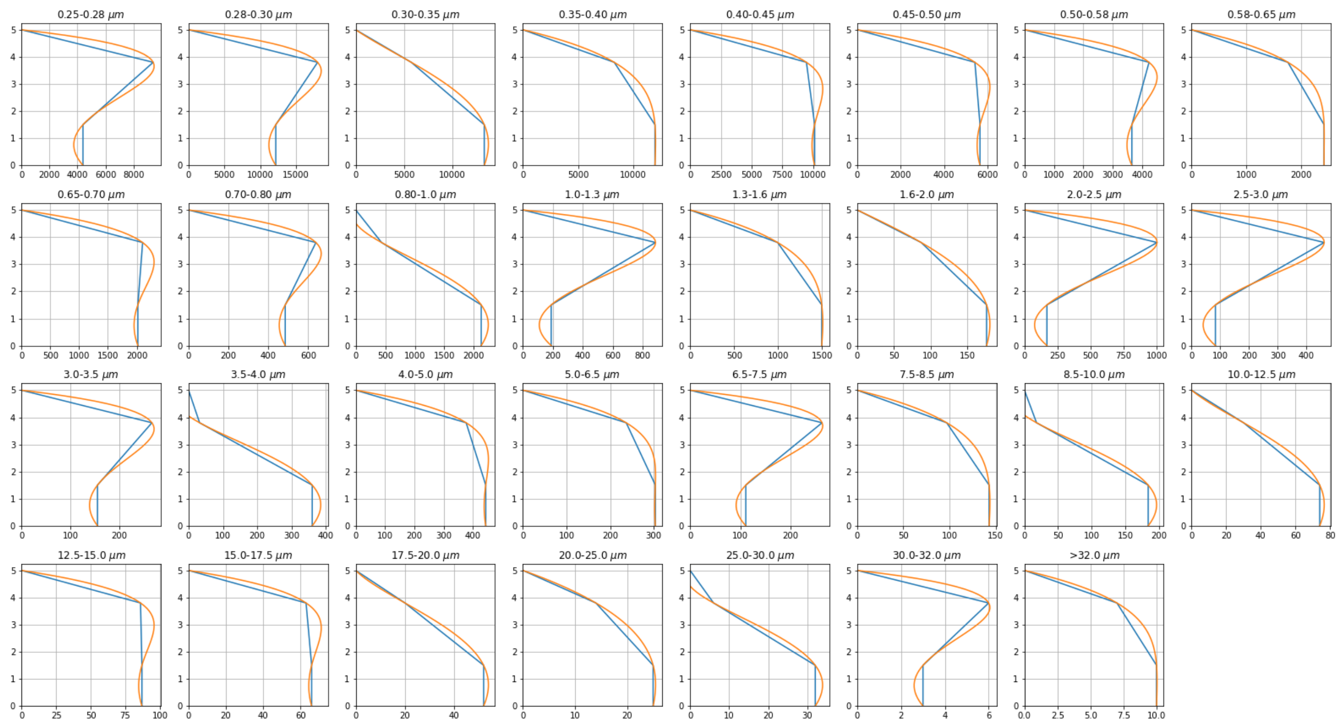

Figure S3. EXP2: Vertical profiles of the particle concentration [particle per litre] for each size bin of the Environmental Dust Monitors; Blue: Measurement; Orange: Polynomial fit; Please note that the scaling of the abscissas vary

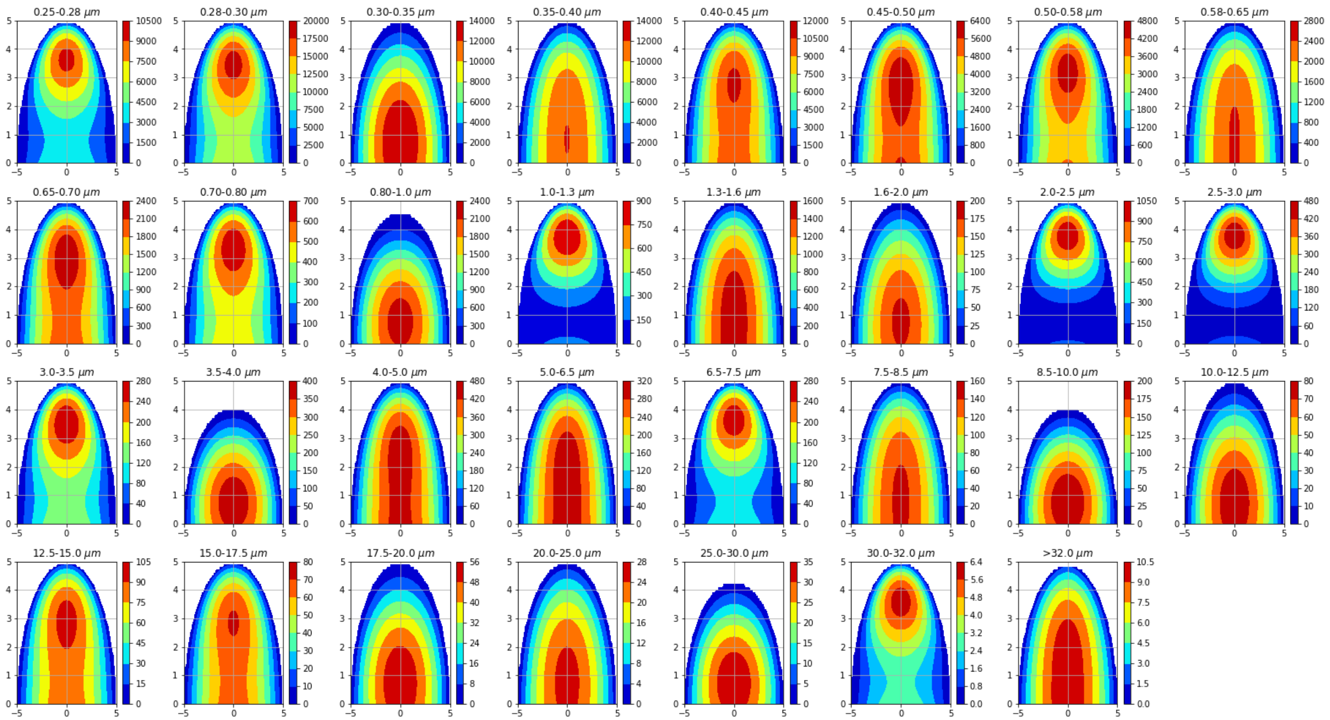

Figure S4. EXP2: Cross-section through the initial particle concentration field [particle per litre] for each size bin of the Environmental Dust Monitors; Please note that the scaling of the colour bar vary

S2 README

```
 ___ _
|_ _| |_ _ __   __ _ ___
 | || __| '_ \ / _` / __|
 | || |_| |_) | (_| \__ \
|___|\__| .__/ \__,_|___/
        |_|
```

In−time particle simulation (Itpas) module in the framework of the COSMO−Model
The in−time wind information and the prognostic turbulent kinetic energy from the COSMO−model are used to calculate the motion of thousands of aerosol particles inside the turbulent atmospheric boundary layer.
Itpas is written as an extension to the weather forecast model COSMO from the German weather service (DWD), so this software container contains beside of Itpas the complete source code of COSMO (V5.4e).

```
 ___           _        _ _       _   _
|_ _|_ __  ___| |_ __ _| | | __ _| |_(_) ___  _ __
 | || '_ \/ __| __/ _` | | |/ _` | __| |/ _ \| '_ \
 | || | | \__ \ || (_| | | | (_| | |_| | (_) | | | |
|___|_| |_|___/\__\__,_|_|_|\__,_|\__|_|\___/|_| |_|
```

Itpas is integrated into the COSMO−model, so the installation follows the same steps as the standard COSMO installation.

1) set the paths in the Fopts file.
   You need an Installation of:
   − The DWD−libgrib (availabe for COSMO users at DWD)
   − grib_api or eccodes
   − NetCDF

2) make (or gmake −j 8 for parallel compiling)

3) The installation worked when the binary cosmo_itpas appears.

```
 _   _
| | | |___  __ _  __ _  ___
| | | / __|/ _` |/ _` |/ _ \
| |_| \__ \ (_| | (_| |  __/
 \___/|___/\__,_|\__, |\___|
                 |___/
```

The NAMELIST "partctl"

```
 &PARTCTL                                                                                  (default)
  nmax_part      = 500000,      ! maximum number of particle in the simulation              (−)
  ischeme        = 1,           ! 1) no turbulence (test mode), 2) TKE turbulence scheme     (1)
  iseed          = 2711         ! seed for the random numbers                                (2711)
  ninc_out_part  = 1,           ! increment of particle output; 1 is every time step         (1)
  heightover     = 'surface'    ! height in startfile is given definde above 'surface' or 'sea'  ('sea')
  startfile_part = './$PFILE',  ! path/of/start/file                                          (−)
  ydir_part      ='${OUTPUT}/', ! path/for/the/output                                         (−)
  lpre_output    = .true.,      ! if true wirte the start position in the netcdf file        (.false.)
  ldrydepo       = .true.       ! activate dry deposition                                    (.true.)
```

```
  lsettling      = .true.       ! activate particle sedimentation                            (.true.)
  vd_constant    = 0.0          ! constant value for the dry deposition velocity.            (0.0)
                                ! [m/s] If 0.0 vd is calculated from the environmental conditions.
```

The namelist has to be stored in the file INPUT_PART

The startfile

A startfile containing the start positions of the trajectories has to be provided.
It is specified by the user via the namelist parameter startfile_part.
It is a text file and its format is strictly defined.
It contains: 3 header lines (no space at the beginning of the lines) and several content lines

```
--- name of the startfile ----------------------------------------------------
time    lon    lat    height    npart    diam     dens      emission
-------------------------------------------------------------------------------
1.00    1.0    2.5    5.0       1200     7.5e-7   2650.0    1.0
5.00    1.0    2.5    5.0        200     7.5e-7   2650.0    0.0
```

- The time is given in hours after model start
- The longitudes are rotated longitudes and can go from -180 to 180 degrees.
  They must be expressed in the same referential (pollon, pollat) than the COSMO grid.
  They can have max. 3 decimal positions.
- The latitudes are rotated latitudes and can go from -90 to 90 degrees.
  They must be expressed in the same referential (pollon, pollat) than the COSMO grid.
  They can have max. 3 decimal positions.
- The height is above see level or above surface [m], dependig on the namelist setting "heightover"
- npart is the number of particles that were emitted at this time and place.
- diam is the diameter of the particle [m], if gas 0.0
- dens is the density of the particle [kg/m3]
- emission is the time in hours that is takes to emit the npart particles
  note: npart/(emission * 3600/dt) need to be an Natural number

COSMO settings

To run the particle model several settings in different COSMO namelists are necessary.

```
1) INPUT_ORG
  &RUNCTL
    lpart=.TRUE.     ! main switch to active the particle model

2) INPUT_PHY
  &PHYCTL
    lforest=.True.,    ! necessary for the calculation of the dry deposition velocity.
    ltur=.TRUE.,       ! we need the turbulence for the turbulent particle transport
    itype_turb=3,      ! TKE based turbulence scheme
    l3dturb=.true.,    ! for best results use the 3d turbulence scheme

3) INPUT_PART as described above
```

```
 _____                           _
| ____|_  ____ _ _ __ ___  _ __ | | ___  ___
|  _| \ \/ / _` | '_ ` _ \| '_ \| |/ _ \/ __|
| |___ >  < (_| | | | | | | |_) | |  __/\__ \
|_____/_/\_\__,_|_| |_| |_| .__/|_|\___||___/
```

```
|_|
```

1) A simple trace – what pathway do the air mass take

```
—— A simple trace ———————————————————————————————————————————
time    lon   lat   height   npart    diam     dens     emission
———————————————————————————————————————————————————————————————
1.00    1.0   2.5   20.0     50000    0.0      0.0      0.0

heightover    = 'surface'
ldrydepo      = .false.
lsettling     = .false.
```

– One hour after model start, 50k air parcels were emitted at once.

2) emitting point source – a chimney

```
—— a chimney ————————————————————————————————————————————————
time    lon   lat   height   npart    diam     dens     emission
———————————————————————————————————————————————————————————————
4.00    1.0   2.5   80.0     115200   0.0      0.0      4.0

heightover    = 'surface'
ldrydepo      = .true.
lsettling     = .false.
vd_constant   = 0.08
```

– We simulate the continuous emission of a gas like tracer.
– 4 hours after the model start, a chimney starts to emit in 80 m attitude.
– The emission goes on for 4 hours, that's 14400 seconds.
– the model uses a time step of (e.q.) 30 seconds,
 so we have (14400/30) 480 time steps in the 4 hours of emission.
– Itpas need to emit at least 1 particle per time step. (If the emission mode is used)
– So npart need to be 480 or an integer multiple of it (480*X)
– Sn the example we use npart = 115200 that's an emission rate of 240 particle per time step
 or 8 particle per second
– Gases can deposit by dry deposition. Therefore a dry deposition velocity is necessary.
 It can be set with vd_constant. The used value in the example 0.08 m/s is a mean value for SO2.

3) a dust plume

```
—— a dust plume ——————————————————————————————————————————————
time    lon   lat   height   npart    diam     dens     emission
———————————————————————————————————————————————————————————————
2.00    1.0   2.5   5.0      1        7.5e-7   2650.0     0.0

heightover    = 'surface'
ldrydepo      = .true.
lsettling     = .true.
```

– for a dust plume, sedimentation is important.
 Therefore need the particle in the start file a diameter and a density.
 And lsettling need to be .true.
– If you want to include a particle size distribution, write a small script
 that defines particle sizes and start position based on your needs.
– An example of how this could be realist can you found here:
 https://github.com/mttfst/dust-bubble