Rocpart **User's Guide**

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Chapter 1

Introduction

1.1 Goal and Scope

The goals of this user's guide are two-fold:

1. To enable users other than the main developer(s) to gain familiarity with the Rocpart module capability.
2. To enable users other than the main developer(s) to install, compile and run Rocpart on various computer systems.

The scope of this user's guide is all the information required to attain the two goals.

1.2 Related Documents

The information contained in this document is supplemented by the following document:

- Rocpart Developer's Guide.
- Rocflo & Rocflu User's Guide.
- Rocfluid_MP Framework Guide.
- Rocinteract Developer's and User's Guides.

1.3 Purpose & Methods

This user's guide describes the main features of Rocpart a Lagrangian Particle Tracking Module. This module is developed to study particles motion with several constituents in a solid propellant rocket motor. The design goal of the module is to implement it with *minimal* modifications to the all-speed compressible fluid solvers, Rocflo & Rocflu.

The present goal focuses on two-phase flow simulation of solid propellant rockets with motion tracking of the large-sized burning particles ($50 - 300\mu m$). A Lagrangian approach has been chosen where individual particles are being tracked over time. This discrete representation will allow to naturally capture the change in the particle constituents as the burning process progresses. The main code characteristics are summarized as follows:

- Stochastic injection model.
- Lagrangian tracking of particle conserved variables, including mass, momentum , energy, and positions.
- Extraction of particle derived variables.
- Explicit time integration.
- Two-way coupling between particle solver and gas solver.
- Flexible expandable framework designed in Fortran-90.
- Highly scalable parallel implementation through block decomposition
  - MPI used for inter-process communications.
  - Non-blocking communications used for optimal performance.

1.4 Governing Equations

Refer to Rocpart & Rocflo Developer's Guides for details on governing equations as well as various models.

Chapter 2

Installation and Compilation

2.1 Installation

2.1.1 Installation of Rocfluid

The procedure outlined below assumes that Rocfluid is to be installed either from the CSAR CVS repository or from a `gzip`ped `tar` file.

2.1.1.1 Installation from CVS Repository

To be able to access the CSAR's CVS repository, set the `CVSROOT` environment variable to (taking the `bash` shell as an example)

```
export CVSROOT=:pserver:<username>@galileo.csar.uiuc.edu:/cvsroot
```

and either open a new terminal or type

```
[user@machine ~]$ source .bashrc
```

Then type

```
[user@machine ~]$ cvs login
```

and hit the `Enter` key at the prompt.

Now move into the directory where you want to install Rocflo. In the following, this is assumed to be `directory`. Then type

```
[user@machine ~/directory]$ cvs co Rocstar/RocfluidMP
```

which will check out the source code for Rocflo from the repository. Assuming these commands to have completed successfully, you are now ready to compile the code for serial computations, and you can proceed to Sec. 2.2 or Sec. 2.3 to compile with Rocflo or Rocflu, respectively.

2.2 Compilation with Rocflo

2.2.1 Overview of Compilation Process

The compilation process for Rocfluid is automatic in the sense that the `Makefile`s determine the machine type and set the suitable compilation options. If you intend to run on IBM, Linux, SGI, or Sun machines, you do not need to modify any `Makefile`s. If you intend to run on other machines, you will need to create your own `Makefile`.

The compilation process consists of two parts. The first part is the actual computation, as described below. The output of the compilation process are several executables:

rfloprep The preprocessing module of Rocflo.

rflomp The flow solver.

rflopost The postprocessing module of Rocflo. (Only compiled if compile with `POST=1`, see below.)

rplagpost The postprocessing module of Rocpart.(Only compiled if compile with `POST=1`, see below.)

The second part consists of copying these executables into your `$(HOME)/bin` directory by typing:

```
[user@machine ~/directory]$ gmake RFLO=1 PLAG=1 install
```

2.2.2 Description of Compilation Options

To compile Rocflo, type the following at the prompt:

```
[user@machine ~/directory]$ gmake RFLO=1 PLAG=1 <options>
```

where the currently supported `<options>` are any of the following:

`PLAG_DEBUG=(0|1)` Deactivates or activates debugging compiler options. Specifying `DEBUG=0`, or leaving out the option altogether, means that no debugging options will be used. Specifying `PLAG_DEBUG=1` will activate debugging options.

`PLAG_MPIDEBUG=(0|1)` Deactivates or activates debugging compiler options under MPI construct. Specifying `DEBUG=0`, or leaving out the option altogether, means that no debugging options will be used. Specifying `PLAG_MPIDEBUG=1` will activate debugging options.

`POST=(0|1)` Deactivates or activates compilation of the postprocessing module rplagpost. Specifying `POST=0`, or leaving out the option altogether, means that rplagpost will not be compiled. Specifying `POST=1` will lead to compilation of rplagpost.

To compile Rocflowith particles using MPI, type the folowing at the prompt:

```
[user@machine ~/directory]$ gmake RFLO=1 PLAG=1 MPI=1
```

To compile Rocflowith particles and smoke, type the folowing at the prompt:

```
[user@machine ~/directory]$ gmake RFLO=1 PLAG=1 PEUL=1
```

To compile Rocflowith particles, smoke and turbulence, type the folowing at the prompt:

```
[user@machine ~/directory]$ gmake RFLO=1 PLAG=1 PEUL=1 TURB=1
```

2.3 Compilation with Rocflu

2.3.1 Overview of Compilation Process

The compilation process for Rocfluid is automatic in the sense that the `Makefile`s determine the machine type and set the suitable compilation options. If you intend to run on IBM, Linux, SGI, Macintosh, or Sun machines, you do not need to modify any `Makefile`s. If you intend to run on other machines, you will need to create your own `Makefile`.

The compilation process consists of two parts. The first part is the actual computation, as described below. The output of the compilation process are several executables:

rfluprep The preprocessing module of Rocflu.

rflump The flow solver.

rflupost The postprocessing module of Rocflu.

The second part consists of copying these executables into your `$(HOME)/bin` directory by typing:

```
[user@machine ~/directory]$ gmake RFLU=1 PLAG=1 install
```

2.3.2 Description of Compilation Options

To compile Rocflo, type the following at the prompt:

```
[user@machine ~/directory]$ gmake RFLU=1 PLAG=1
```

Chapter 3

Execution

This chapter contains detailed information on the command-line arguments and input and output files of Rocflo, rplagpost, and Rocflu.

3.1 Rocflo

3.1.1 Command-Line Arguments

For serial computations, Rocflo is invoked by typing

```
rflomp <casename> <verbosity>
```

where

`<casename>` is a character string used to label the input and output files.

`<verbosity>` is an integer indicating the desired verbosity level of Rocflo. The verbosity level can take the following values:

- `0` No output. Rocflo will not write any information to standard output.
- `1` Low level of output. Rocflo will write some information to standard output.
- `2` High level of output. Rocflo will write detailed information to standard output.

For parallel computations, Rocflo is invoked by typing

```
mpirun -np <number_of_processors> rflomp <casename> <verbosity>
```

3.1.2 Input Files

The following input files are read by Rocflo:

- An input file called `<casename>.inp`.
- A grid file in Rocflo format.

- A boundary condition file. The name of the file is `<casename>.bc`.
- A topology file. The name of the file is `<casename>.top`.
- A flow solution file in Rocflo format. The name of the flow solution file is specified for an unsteady computation (refer to Rocflo User's Guide).
- A particle solution file in Rocpart format. The name of the particle solution file is `<casename>.plag_sola_0.00000E+00` for ASCII formatted file and `<casename>.plag_solb_0.00000E+00` for binary formatted file.

3.1.3 Output Files

The following input files are written by Rocflo:

- A flow solution file in Rocflo format.
- A particle solution file in Rocpart format. The name of the particle solution file is `<casename>.plag_sola_<stamp>` for ASCII formatted file and `<casename>.plag_solb_<stamp>` for binary formatted file.

3.2 rplagpost with Rocflo

3.2.1 Command-Line Arguments

For serial computations, rplagpost is invoked by typing

```
plagpost <casename> <time> <format>
```

where

`<casename>` is a character string used to label the input and output files.

`<time>` is a variable indicating the time from which the solution file is to be read.

`<format>` is an integer indicating the type of output. `<format>` can take the following values:

1 Write solution output file in generic binary format.

2 Write solution output file in Tecplot binary format.

3 Write solution output file in Tecplot ASCII format.

Currently only option 3 is supported

3.2.2 Input Files

No input files are currently written by rplagpost:

3.2.3 Output Files

The following output files are written by rplagpost:

- A file in Tecplot format called <casename>.plag_<stamp>.plt.

3.3 Rocflu

3.3.1 Command-Line Arguments

For serial computations, Rocflu is invoked by typing

```
rflumap -c <casename> -m <type> -p <procs> -r <regions> -v <verbosity>

rflupart -c <casename> -v <verbosity>

rfluinit -c <casename> -v <verbosity>

rflump -c <casename> -v <verbosity>

rflupost -c <casename> -s <timestamp> -v <verbosity>
```

For parallel computations, Rocflu is invoked by typing

```
rflumap -c <casename> -m <type> -p <procs> -r <regions> -v <verbosity>

rflupart -c <casename> -v <verbosity>

rfluinit -c <casename> -v <verbosity>

mpirun -np <procs> rflump -c <casename> -v <verbosity>

rflupost -c <casename> -s <timestamp> -v <verbosity>
```

where

<casename> is a character string used to label the input and output files.

<verbosity> is an integer indicating the desired verbosity level of Rocflu. The verbosity level can take the following values:

- 0 No output. Rocflu will not write any information to standard output.
- 1 Low level of output. Rocflu will write some information to standard output.
- 2 High level of output. Rocflu will write detailed information to standard output.

<timestamp> is a real indicating the desired timestamp to create the visualization files.

<nprocs> is the number of processors.

<regions> is the number of regions.

The preparation tools (rflumap,rflupart, & rfluinit) generate all the pertinent files to perform a calculation with particles that are ran by rflump. The postprocessing tool (rflupost) creates the pertinent files for visualization purposes. Further details can be found in the Rocflu Developer's and User's Guides.

3.3.2 Input Files

The following input files are read by Rocflu:

- An input file called <casename>.inp.
- A grid file in Rocflu format.
- A boundary condition file. The name of the file is <casename>.bc.
- A topology file. The name of the file is <casename>.top.
- A flow solution file in Rocflu format. The name of the flow solution file is specified for an unsteady computation (refer to Rocflu User's Guide).
- A particle dimension file in Rocpart format. The name of the particle solution file is <casename>.pdim_00000_0.00000E+00.It is always in ASCII format.
- A particle solution file in Rocpart format. The name of the particle solution file is <casename>.plag_sola_00000_0.00000E+00 for ASCII formatted file and <casename>.plag_sol_00000_0.00000E+00 for binary formatted file.

3.3.3 Output Files

The following input files are written by Rocflu:

- A flow solution file in Rocflu format.
- A particle dimension file in Rocpart format. The name of the particle solution file is <casename>.pdim_region>_<stamp>.It is always in ASCII format.
- A particle solution file in Rocpart format. The name of the particle solution file is <casename>.plag_sola_<region>_<stamp> for ASCII formatted file and <casename>.plag_sol_<region>_<stamp> for binary formatted file.

Chapter 4

Rocpart File Format Specifications

The files read and written by Rocflo, Rocflu, and rplagpost are described in this chapter. Note that all files share a user-specified string, the so-called 'case name'.

4.1 Input File

The input file is called `<casename>.inp`. The input file is divided into sections. Each section contains several lines, each of which consists of a keyword and a value, as shown below.

```
# SECTION_NAME
KEYWORD_1         VALUE_1
KEYWORD_2         VALUE_2
KEYWORD_3         VALUE_3
#
```

Comments may be inserted after the specification of the values; they are ignored by the routines reading the input file.

The Input file section pertinent to Rocpart variables starts with #DISPART #DISPART_NCONT and Rocinteract specific keywords. The detailed description of these sections and their associated keywords is as follows

4.1.1 `DISPART` Section

The `DISPART` section contains the following keywords:

`BLOCK` Specifies what regions are activate for Rocpart. It is of type INTEGER and is usually set as (`0 0`). This means that the conditions set below apply to all regions. This option could be used to deactivate specific regions or change specific options for individual regions. This option is not needed when running with Rocflu.

`USED` Specifies if the module is used. It is of type INTEGER and takes values of 0 or 1. A value of 0 means the module is not used.

NPCLSTOT Specifies the maximum number of particles. to be evolved in each region. It is an INTEGER with minimum value of 0. If this number is exceeded, the computation crashes.

EJECMODEL Specifies the ejection model to be invoked. It is an INTEGER currently taking either a value of 1 (PLAG_EJEC_MODEL1) for a lognormal distribution or 2 (PLAG_EJEC_CRE) for a skewed clipped logarithmic distribution.

INJCVELRATIO Specifies the injection velocity ratio between the particle and the mixture. It is of RFREAL with minimum value of 0.0_RFREAL.

SPLOAD Specifies the superparticle loading. It is of type RFREAL with a default value of 1.0_RFREAL.

INJCBETA Specifies the injection time coefficient. It is of type RFREAL and usually is set to a default value of 1.0_RFREAL. Customarily, INJCBETA is set to 2 order of magnitude larger than SPLOAD when using EJECMODEL set to PLAG_EJEC_MODEL1. For example, SPLOAD= 10^3, INJCBETA= 10^5. For EJECMODEL set to PLAG_EJEC_CRE (2), INJCBETA should be set to 1.

INJCDIAMDIST Specifies the injection model for the diameter distribution to be invoked. It is an INTEGER currently taking the following values of 1 (PLAG_INJC_LOGNORM) for a log-normal distribution , 2 (PLAG_INJC_LOGSKWD) for a skewed clipped logarithmic distribution, 3 (PLAG_INJC_PDF) for a pdf-based distribution. The third option requires a file named, <casename>.plag_injcpdf. The default is set to 1 (PLAG_INJC_LOGNORM).

INJCDIAMMEAN Specifies the mean particle diameter at injection. It is of type RFREAL.

INJCDIAMMIN Specifies the minimum particle diameter at injection. It is of type RFREAL and is active for INJCMODEL=2.

INJCDIAMMAX Specifies the maximum particle diameter at injection. It is of type RFREAL and is active for INJCMODEL=2.

INJCSTDDEV Specifies the standard deviation of the particle diameter at injection. It is of type RFREAL with a minimum value of 0.0_RFREAL.

INTRPLMIXTMODEL Specifies the interpolation model type for the mixture properties. It is of type INTEGER taking values of ZEROTH_ORDER (0), FIRST_ORDER (1), or SECOND_ORDER (2). Current support is for ZEROTH_ORDER.

NPCLSBUFFTOT Specifies the total buffer size for patches used in communication algorithm. It is of type INTEGER with minimum value of 0. If this number is exceeded, the computation crashes.

BREAKUPMODEL Specifies the breakup model. It is an INTEGER currently taking either a value of 0 (PLAG_BREAKUP_NOMODEL) for no breakup model or 1 (PLAG_BREAKUP_MODEL1) for a simplified Weber-based breakup model.

BREAKUPFAC Specifies the breakup factor. It is an REAL currently with typical value of 2.

BREAKUPWEBSWI Specifies the switch for the breakup model. It is an INTEGER currently taking either a value of 0 (PLAG_BREAKUP_NOWEBSWI) for a non-active switch or 1 (PLAG_BREAKUP_WEBSWI1) for an active switch.

4.1.2 DISPART_NCONT Section

The DISPART_NCONT section contains the following keywords:

NCONT Specifies the total number of constituents that make up the particle. It is of type INTEGER with no default value and has to be at least 1.

MATERIALNAME Specifies the material name to point to.

injcMassFluxRatio Specifies the mass flux ratio of each constituent. It is a RFREAL array with minimum dimension of 1.

4.1.3 DISPART_INIT Section

The DISPART_INIT section is only active with Rocflu and contains the following keywords:

FLAG Specifies the flag type for the particle initialization. It is of type INTEGER and takes values of 1 for scratch or 2 for random state.

NPCLSRAND Specifies the number of initial random particles

NUMBER has a dual function.

- For FLAG set to 1, it represents the number of particles to generate from scratch.
- For FLAG set to 4, it takes a value of 2 corresponding to the minimum and maximum values of positions, diameter, temperature, superparticle loading, and velocities.

- When FLAG set to 1, for certain value of NUMBER, the following variables will be included iniPosX, iniPosY, iniPosZ, iniDiam, iniTemp, iniSpLoad, iniVelX, iniVelY, iniVelZ.
- When FLAG set to 4, the first line includes iniRandDiamMin, iniRandTempMin, iniRandSpLoadMin, iniRandXMin, iniRandYMin, and iniRandZMin; while the second line includes: iniRandDiamMax,iniRan
iniRandSpLoadMax, iniRandXMax, iniRandYMax, and iniRandZMax.

The material definitions are specified in #MATERIAL Section. Further, these keywords are active on all regions.

4.1.4 INRT_DEFAULT Section

The INRT_DEFAULT specifies the activeness or passiveness of each state during the computation based on block numbers. Further details are given in Rocinteract User's Guide.

4.1.5 INRT_DRAG Section

The INRT_DRAG section specifies the momentum drag model and contains the following keywords:

BLOCK Specifies what regions are activate for Rocpart. It is of type INTEGER and is usually set as (0 0). This means that the conditions set below apply to all regions. This option could be used to deactivate specific regions or change specific options for individual regions.

USED Specifies if the module is used. It is of type INTEGER and takes values of 0 or 1. A value of 0 means the module is not used.

MODEL Specifies the drag model to be invoked. It is an INTEGER currently taking either a value of 1 for Stokes model or 2 for Schiller-Naumann correlation. The default value is 2.

4.1.6 INRT_HEAT_TRANSFER_NONBURN Section

The INRT_HEAT_TRANSFER_NONBURN section specifies the thermal drag model and contains the following keywords:

BLOCK Specifies what regions are activate for Rocpart. It is of type INTEGER and is usually set as (0 0). This means that the conditions set below apply to all regions. This option could be used to deactivate specific regions or change specific options for individual regions.

USED Specifies if the module is used. It is of type INTEGER and takes values of 0 or 1. A value of 0 means the module is not used.

MODEL Specifies the thermal drag model to be invoked. It is an INTEGER currently taking either a value of 1 for Stokes model or 2 for Ranz-Marshall correlation. The default value is 2.

4.1.7 INRT_SCOURING Section

The INRT_SCOURING section specifies the scouring model and contains the following keywords:

BLOCK Specifies what regions are activate for Rocpart. It is of type INTEGER and is usually set as (0 0). This means that the conditions set below apply to all regions. This option could be used to deactivate specific regions or change specific options for individual regions.

USED Specifies if the module is used. It is of type INTEGER and takes values of 0 or 1. A value of 0 means the module is not used.

COEF[n] Specifies the scouring coefficient for Smoke type [n]. It is a REAL currently taking either a value of a maximum of 1.0. The default value is 1.0. Typical values are 0.25. n is an INTEGER starting at 1.

Note that the number in COEF[n] depends on the total number of smoke types being evolved. Details are provided in Rocinteract User's Guide.

4.1.8 INRT_BURNING Section

The INRT_BURNING section specifies the burning model and contains the following keywords:

BLOCK Specifies what regions are activate for Rocpart. It is of type INTEGER and is usually set as (0 0). This means that the conditions set below apply to all regions. This option could be used to deactivate specific regions or change specific options for individual regions.

USED Specifies if the module is used. It is of type INTEGER and takes values of 0 or 1. A value of 0 means the module is not used.

MATERIAL_IN Specifies the string of the material that burns. It is a CHARACTER with typical values ALUMINUM.

MATERIAL_OUT Specifies the string of the material created by the burning process. It is a CHARACTER with typical values ALUMINUM_OXIDE.

MATERIAL_OX Specifies the string of the material used to oxidize. It is a CHARACTER with typical values OXIDIZER.

MODEL Specifies the burning model to be invoked. It is an INTEGER currently taking a value of 1 for Becsktead model.

OX_USED Specifies whether to use oxidizer field. It is an INTEGER currently taking a value of 0 or 1. The default value is 0.

VAPOR_METHOD Specifies whether to use vapor method for full heat release. It is an INTEGER currently taking a value of 0 or 1. The default value is 0.

HEAT_COEF Specifies the fraction of actual energy released due to burning. It is a REAL currently taking values between 0.0 or 1.0. The default value is 1.0.

MFRC_PLAG Specifies the fraction of Al2O3 going back to the particle. It is a REAL currently taking values between 0.0 or 1.0. The default value is 0.0.

MFRC_PEUL[n] Specifies the fraction of Al2O3 going back to smoke of type [n].It is a REAL currently taking values between 0.0 or 1.0. The default value is 0.0.

Note that the number in MFRC_PEUL[n] depends on the total number of smoke types being evolved. Details are provided in Rocinteract User's Guide.

4.2 Output Files for Rocflo

The output files generated by Rocpart are created at the same frequency as the solution files created by Rocflo. The file created has the following nomenclature casename.pcls_sol[a,b]_*time*. The format mimics that developed for Rocflo where arrays are loaded into intermediate array file (named aivFile,arvFile,cvFile). In general, Rocpart saves aiv,arv,cv for the PLAG datastructure. While for the Tile datastructure, it saves cv and dv(DV_TILE_TIMEFCTR,:). If a region has no particles in it, only the number of particles is written. Similar process is undertaken for the tiles. The output file for the Lagrangian particles is written (and read) as follows:

```
time
nDimPlag, nextIdNumber
aivFile
arvFile
cvFile

nDimTile
cvFile
dvFile
```

where time is the physical time at which this solution prevails, nDimPlag is the number of particles in the computational region, and nDimTile is the number of injecting tiles on that computational region. The remaining variables are described in details in the Rocpart Developer's Guide.

4.3 Restart Capabilities

The restart capability follows the Rocflo mechanism and is described in Rocflo User's guide. To start Rocpart computations with a "fresh" flow field the restart file casename.plag_sola_0.00000E+00 has to be as follows:

```
0.0E+0
1 0 0
1 0
```

4.4 Output Files for Rocflu

The files pertinent to Rocpart are written once the condition satisfied by writeTime is satisfied. Hence,it follows closely the solution write-up of Rocflu (see Rocflu Developer's Guide). This stage is initiated in the subroutine (PLAG_RFLU_WriteSolution_ASCII
or PLAG_RFLU_WriteSolution_Binary). For restart, the file is read from the construct of
PLAG_RFLU_ReadSolution_ASCII
or PLAG_RFLU_ReadSolution_Binary.

The output files generated by Rocpart are created at the same frequency as the solution files created by Rocflu. The file created has the following nomenclature casename.plag_sol[a]_*region_time*. The format mimics that developed for Rocflo where arrays are loaded into intermediate array file (named aivFile,arvFile,cvFile). In general, Rocpart saves aiv,arv,cv for the PLAG datastructure. While for the Tile datastructure, it saves cv and dv(DV_TILE_TIMEFCTR,:). If a region has no particles in it, only the number of particles is written. Similar process is undertaken for the tiles. The output file for the Lagrangian particles is written (and read) as follows:

```
# ROCPART dimensions file
# Actual number of particles
       nDimPlag
# Maximum number of particles
    nDimPlagMax
# Number of constituents
       nCont
# Next particle identifier
       nextIdNumber
# End

# ROCFLU particle file
# Precision and range
      15     307
# Physical time
 time
# Dimensions
       nDimPlag      nVars
```

```
# Particle x-momentum
   cv(CV_PLAG_XMOM,:)
# Particle y-momentum
  cv(CV_PLAG_YMOM,:)
# Particle z-momentum
   cv(CV_PLAG_ZMOM,:)
# Particle energy
   cv(CV_PLAG_ENER,:)
# Particle x-location
   cv(CV_PLAG_XPOS,:)
# Particle y-location
   cv(CV_PLAG_YPOS,:)
# Particle z-location
   cv(CV_PLAG_ZPOS,:)
# Particle vapor energy
   cv(CV_PLAG_ENERVAPOR,:)
# Particle mass
   cv(CV_PLAG_LAST+1,:)
# Particle mass
   cv(CV_PLAG_LAST+nCont,:)
# Particle superloading
   arv(ARV_PLAG_SPLOAD,:)
# Particle initial identifier
   aiv(AIV_PLAG_PIDINI,:)
# Particle initial region
   aiv(AIV_PLAG_REGINI,:)
# Particle cell
   aiv(AIV_PLAG_ICELLS,:)
# Patch data

# End
```

where `time` is the physical time at which this solution prevails, `nDimPlag` is the number of particles in the computational region, `nDimPlagMax` is the maximumnumber of particles in the computational region `nextIdNumber` is a counter that keeps track of the particle id's and `nVars` is the number of variables.

Chapter 5

Examples and Test Problems

This chapter provides several test case examples to run Rocflo with Lagrangian particles under distinct modes of operations. Test cases based on single and multiple regions are outlined.

5.1 ONERA C0 Numerical Experiment with Passive Particles

The ONERA C0 example is described in various papers and consists of an injecting bottom wall, a top symmetry plane, an exit plane and a non-slip wall. The example file can be found in CVS in the following directory path RocfluidMP/calcs/application/onerac0-mp/rocflo/plag

5.1.1 Input File

```
! Input file for C0 - viscous

! mapping of blocks to processors -----------------------------------------------

# BLOCKMAP
NBLOCKS   0      ! no. of blocks per processor (0=automatic mapping)
#

! grid/solution format ----------------------------------------------------------

# FORMATS
GRID      0      ! 0=Plot3D ASCII, 1=Plot3D binary, 2=HDF
SOLUTION  0      ! 0=ASCII, 1=binary, 2=HDF
#

! Random number generator--------------------------------------------------------

# RANDOM
SEED_OFFSET  0   ! Offset for seed of RNG (default = 0, otherwise: 1,2,3,etc)
#

! viscous/inviscid flow ----------------------------------------------------------

# FLOWMODEL
```

```
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL     1      ! 0=inviscid (Euler), 1=viscous (Navier-Stokes)
MOVEGRID  0      ! moving grid (0=no, 1=yes)
#

! reference values ------------------------------------------------------------

# REFERENCE
ABSVEL   1.0     ! reference velocity
DENS     1.0     ! reference density
CP       1004.5  ! specific heat coeff. at constant pressure [J/kgK]
GAMMA    1.4     ! ratio of specific heats
LENGTH   1.0     ! reference length
RENUM    5.0E04  ! reference Reynolds number
#

! probe -----------------------------------------------------------------------

# PROBE
NUMBER   0
#

! forces ----------------------------------------------------------------------

# FORCES
TYPE     1       ! 0=no forces calculated, 1=pressure forces, 2=1+viscous forces
#

! material definitions --------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#
```

```
# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#

! multi-physics modules: ------------------------------------------------------

# TURBULENCE
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=laminar, 1=...
#

# SPECIES
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=perfect gas, 1=...
#

# CONPART
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

# DISPART
BLOCK    0  0    ! applies to block ... (0 0 = to all)
USED     1       ! 0=module not used
NPCLSTOT        10000     ! Total Number of DisPart
EJECMODEL       1         ! Ejection Model
INJCVELRATIO    0.0       ! Injection Velocity Ratio
SPLOAD          5.00E+2   ! SuperParticle Loading
INJCBETA        5.00E+5   ! Injection beta Coefficient
INJCDIAMDIST    1         ! Injection Diameter Distribution Model
INJCDIAMMEAN    10.0E-06  ! Injection Mean Diameter
INJCDIAMMIN     5.0E-06   ! Injection Mean Diameter
INJCDIAMMAX     100.0E-06 ! Injection Mean Diameter
INJCSTDDEV      0.0       ! injection Standard Deviation
INTRPLMIXTMODEL 0         ! Interpolation Order for Mixture
NPCLSBUFFTOT    1000      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0         ! Breakup Model
BREAKUPFAC      2.0       ! Breakup Factor
BREAKUPWEBSWI   0         ! Breakup Weber Switch
#

# DISPART_NCONT
NCONT   2
```

```
ALUMINUM         0.162  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.018  ! MaterialName, injcMassRatio
#

# INRT_DEFAULT
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   0    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
#

# INRT_DRAG
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#

# RADIATION
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

! time-stepping control ------------------------------------------------------

# TIMESTEP
FLOWTYPE   1      ! 0=steady flow, 1=unsteady flow

! if FLOWTYPE=0
STARTITER     0   ! current iteration
MAXITER    20000  ! max. number of iterations
RESTOL     1.E-5  ! max. density residual to stop iterations
WRIITER    2000   ! offset between iterations to store solution
PRNITER    1      ! offset between iterations to print convergence

! if FLOWTYPE=1
TIMESTEP   1.0E-5 ! max. physical time step [s]
STARTTIME  0.0    ! current time
MAXTIME    6.0E-3 ! max. time simulated [s]
WRITIME    2.0E-3 ! time offset [s] to store solution
PRNTIME    1.0E-5 ! time offset [s] to print convergence
#

! numerics -------------------------------------------------------------------

# MULTIGRID
START    1       ! at which grid level to start (>0; 1=finest grid)
```

```
CYCLE    0       ! 0=no MG, 1=V-cycle, 2=W-cycle
REFINE   99999   ! no. of iterations before switching to next finer grid
#

# NUMERICS
BLOCK    0  0    ! applies to block ... (0 0 = to all)
CFL      7.5     ! CFL number
SMOOCF   1.0     ! coefficient of implicit residual smoothing (<0 - no smooth.)
DISCR    0       ! type of space discretization (0=central, 1=Roe, 2=MAPS)
K2       0.0     ! dissipation coefficient k2 (if discr=0)
1/K4     128.    ! dissipation coefficient 1/k4 (if discr=0)
ORDER    2       ! 1=first-order, 2=second-order, 4=fourth-order
LIMFAC   5.0     ! limiter coefficient (if discr=1)
ENTROPY  0.05    ! entropy correction coefficient (if discr=1)
#
```

5.1.2 Single-Block `.top` File

```
# topology file for C0 - 1 block
#
 1      ! total no. of blocks
 1  1   ! block, no. of grid levels
 6  100  50  2            ! no. of patches, icells, jcells, kcells
 70  1   1   50    1    2    0   0   0   0   0   0   0
 20  2   1   50    1    2    0   0   0   0   0   0   0
100  5   1  100    1   50    0   0   0   0   0   0   0
100  6   1  100    1   50    0   0   0   0   0   0   0
100  4   1    2    1  100    0   0   0   0   0   0   0
 90  3   1    2    1  100    0   0   0   0   0   0   0
```

5.1.3 Boundary Condition `.bc` File

```
! File with boundary conditions for C0

# BC_SLIPW
BLOCK     0  0   ! applies to block ... (0 0 = to all)
PATCH     0  0   ! applies to patch ... (0 0 = to all patches BLOCK)
EXTRAPOL  1      ! order of extrapolation to dummy cells (0 or 1)
MAXCHANGE 1.0    ! controls maximum change in variable
#

! ----------------

# BC_NOSLIP
BLOCK     0  0   ! applies to block ... (0 0 = to all)
PATCH     0  0   ! applies to patch ... (0 0 = to all patches from above range of blocks)
ADIABAT   1      ! wall boundary condition: 0=T given, 1=adiabatic
TWALL     303.0  ! wall temperature [K] (if adiabat=0 and distrib=0)
#
```

```
! ----------------


# BC_INJECT
BLOCK     0  0   ! applies to block ... (0 0 = to all)
PATCH     0  0   ! applies to patch ... (0 0 = to all patches of BLOCK)
EXTRAPOL  1      ! order of extrapolation to dummy cells (0 or 1)
DISTRIB   0      ! single value (=0) or distribution (=1)
MFRATE    2.42   ! mass flow rate [kg/(m^2*s)] (if distrib=0)
TEMP      303.   ! injection temperature [K] (if distrib=0)
MAXCHANGE 1.0    ! controls maximum change in variables
#

! ----------------

# BC_OUTFLOW
BLOCK    0  0    ! applies to block ... (0 0 = to all)
PATCH    0  0    ! applies to patch ... (0 0 = to all patches of BLOCK)
TYPE     1       ! 0=supersonic only, 1=subsonic only, 2=mixed
DISTRIB  0       ! single value (=0) or distribution (=1)
PRESS    1.5E+5  ! static pressure [Pa] (if type=1 or 2)
#
```

5.2 ONERA C0 Numerical Experiment with Active Non-Burning Particles

5.2.1 Input File

```
! Input file for C0 - viscous

! mapping of blocks to processors -----------------------------------------------

# BLOCKMAP
NBLOCKS   0      ! no. of blocks per processor (0=automatic mapping)
#

! grid/solution format ----------------------------------------------------------

# FORMATS
GRID      0      ! 0=Plot3D ASCII, 1=Plot3D binary, 2=HDF
SOLUTION  0      ! 0=ASCII, 1=binary, 2=HDF
#

! Random number generator-------------------------------------------------------

# RANDOM
SEED_OFFSET  0   ! Offset for seed of RNG (default = 0, otherwise: 1,2,3,etc)
#
```

```
! viscous/inviscid flow ------------------------------------------------------

# FLOWMODEL
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL     1      ! 0=inviscid (Euler), 1=viscous (Navier-Stokes)
MOVEGRID  0      ! moving grid (0=no, 1=yes)
#

! reference values ------------------------------------------------------------

# REFERENCE
ABSVEL   1.0     ! reference velocity
DENS     1.0     ! reference density
CP       1004.5  ! specific heat coeff. at constant pressure [J/kgK]
GAMMA    1.4     ! ratio of specific heats
LENGTH   1.0     ! reference length
RENUM    5.0E04  ! reference Reynolds number
#

! probe -----------------------------------------------------------------------

# PROBE
NUMBER   0
#

! forces ----------------------------------------------------------------------

# FORCES
TYPE     1       ! 0=no forces calculated, 1=pressure forces, 2=1+viscous forces
#

! material definitions --------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.69   ! surface tension
#

# MATERIAL
NAME   ALUMINUM_OXIDE
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
#

# MATERIAL
NAME   OXIDIZER
```

```
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS  1.0   ! surface tension
#

! multi-physics modules: ------------------------------------------------------

# TURBULENCE
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=laminar, 1=...
#

# SPECIES
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=perfect gas, 1=...
#

# CONPART
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

# DISPART
BLOCK    0  0    ! applies to block ... (0 0 = to all)
USED     1       ! 0=module not used
NPCLSTOT        10000     ! Total Number of DisPart
INJCMODEL       1         ! Injection Model
INJCVELRATIO    0.0       ! Injection Velocity Ratio
SPLOAD          5.00E+2   ! SuperParticle Loading
INJCDIAMMEAN    10.0E-06  ! Injection Mean Diameter
INJCDIAMMIN     5.0E-06   ! Injection Mean Diameter
INJCDIAMMAX     100.0E-06 ! Injection Mean Diameter
INJCSTDDEV      0.0       ! injection Standard Deviation
INJCTIMECOEFF   5.00E+5   ! injection Time Coefficient
INTRPLMIXTMODEL 0         ! Interpolation Order for Mixture
NPCLSBUFFTOT    1000      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0         ! Breakup Model
BREAKUPFAC      2.0       ! Breakup Factor
BREAKUPWEBSWI   0         ! Breakup Weber Switch
#

# DISPART_NCONT
NCONT   2
ALUMINUM         0.162  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.018  ! MaterialName, injcMassRatio
#

# INRT_DEFAULT
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
```

```
PLAG_ACTV   1    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
#

# INRT_DRAG
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#

# RADIATION
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

! time-stepping control ----------------------------------------------------

# TIMESTEP
FLOWTYPE   1      ! 0=steady flow, 1=unsteady flow

! if FLOWTYPE=0
STARTITER     0   ! current iteration
MAXITER    20000  ! max. number of iterations
RESTOL     1.E-5  ! max. density residual to stop iterations
WRIITER    2000   ! offset between iterations to store solution
PRNITER    1      ! offset between iterations to print convergence

! if FLOWTYPE=1
TIMESTEP   1.0E-5 ! max. physical time step [s]
STARTTIME  0.0    ! current time
MAXTIME    6.0E-3 ! max. time simulated [s]
WRITIME    2.0E-3 ! time offset [s] to store solution
PRNTIME    1.0E-5 ! time offset [s] to print convergence
#

! numerics -----------------------------------------------------------------

# MULTIGRID
START    1       ! at which grid level to start (>0; 1=finest grid)
CYCLE    0       ! 0=no MG, 1=V-cycle, 2=W-cycle
REFINE   99999   ! no. of iterations before switching to next finer grid
#

# NUMERICS
BLOCK    0  0    ! applies to block ... (0 0 = to all)
CFL      7.5     ! CFL number
```

```
SMOOCF   1.0     ! coefficient of implicit residual smoothing (<0 - no smooth.)
DISCR    0       ! type of space discretization (0=central, 1=Roe, 2=MAPS)
K2       0.0     ! dissipation coefficient k2 (if discr=0)
1/K4     128.    ! dissipation coefficient 1/k4 (if discr=0)
ORDER    2       ! 1=first-order, 2=second-order, 4=fourth-order
LIMFAC   5.0     ! limiter coefficient (if discr=1)
ENTROPY  0.05    ! entropy correction coefficient (if discr=1)
#
```

5.3 ONERA C0 Numerical Experiment with Active Burning Particles

5.3.1 Input File

```
! Input file for C0 - viscous

! mapping of blocks to processors ------------------------------------------------

# BLOCKMAP
NBLOCKS   0      ! no. of blocks per processor (0=automatic mapping)
#

! grid/solution format ----------------------------------------------------------

# FORMATS
GRID      0      ! 0=Plot3D ASCII, 1=Plot3D binary, 2=HDF
SOLUTION  0      ! 0=ASCII, 1=binary, 2=HDF
#

! Random number generator--------------------------------------------------------

# RANDOM
SEED_OFFSET  0   ! Offset for seed of RNG (default = 0, otherwise: 1,2,3,etc)
#

! viscous/inviscid flow ----------------------------------------------------------

# FLOWMODEL
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL     1      ! 0=inviscid (Euler), 1=viscous (Navier-Stokes)
MOVEGRID  0      ! moving grid (0=no, 1=yes)
#

! reference values ---------------------------------------------------------------

# REFERENCE
ABSVEL   1.0     ! reference velocity
DENS     1.0     ! reference density
CP       1004.5  ! specific heat coeff. at constant pressure [J/kgK]
```

```
GAMMA    1.4     ! ratio of specific heats
LENGTH   1.0     ! reference length
RENUM    5.0E04  ! reference Reynolds number
#

! probe -------------------------------------------------------------------

# PROBE
NUMBER   0
#

! forces ------------------------------------------------------------------

# FORCES
TYPE     1       ! 0=no forces calculated, 1=pressure forces, 2=1+viscous forces
#

! material definitions -----------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#

# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#
```

```
! multi-physics modules: ------------------------------------------------------

# TURBULENCE
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=laminar, 1=...
#

# SPECIES
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=perfect gas, 1=...
#

# CONPART
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

# DISPART
BLOCK    0  0    ! applies to block ... (0 0 = to all)
USED     1       ! 0=module not used
NPCLSTOT        10000     ! Total Number of DisPart
EJECMODEL       1         ! Ejection Model
INJCVELRATIO    0.0       ! Injection Velocity Ratio
SPLOAD          5.00E+2   ! SuperParticle Loading
INJCBETA        5.00E+5   ! Injection beta Coefficient
INJCDIAMDIST    1         ! Injection Diameter Distribution Model
INJCDIAMMEAN    10.0E-06  ! Injection Mean Diameter
INJCDIAMMIN     5.0E-06   ! Injection Mean Diameter
INJCDIAMMAX     100.0E-06 ! Injection Mean Diameter
INJCSTDDEV      0.0       ! injection Standard Deviation
INTRPLMIXTMODEL 0         ! Interpolation Order for Mixture
NPCLSBUFFTOT    1000      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0         ! Breakup Model
BREAKUPFAC      2.0       ! Breakup Factor
BREAKUPWEBSWI   0         ! Breakup Weber Switch
#

# DISPART_NCONT
NCONT   2
ALUMINUM         0.162  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.018  ! MaterialName, injcMassRatio
#

# INRT_DEFAULT
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   1    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
PEUL1_ACTV  0    ! (0=Passive, 1=Active) Activeness of Smoke type 1
PEUL2_ACTV  0    ! (0=Passive, 1=Active) Activeness of Smoke type 2
PEUL3_ACTV  0    ! (0=Passive, 1=Active) Activeness of Smoke type 3
```

```
#

# INRT_DRAG
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#

# INRT_SCOURING
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=interaction not used (default: 1)
COEF1  0.25      ! Scouring Coefficient for Smoke type 1 (default: 1.0)
COEF2  0.0       ! Scouring Coefficient for Smoke type 2 (default: 1.0)
#

# INRT_BURNING
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=interaction not used (default: 1)
MATERIAL_IN   ALUMINUM       ! material that burns
MATERIAL_OUT  ALUMINUM_OXIDE ! material created by the burning process
MATERIAL_OX   OXIDIZER       ! material used to oxidize
MODEL  1         ! (1=Beckstead correlation) (1 is default)
OX_USED    0     ! Whether to use oxidizer field (0=no,1=yes) (default: 0)
HEAT_COEF  0.20  ! Fraction of Actual Energy Released (default: 1.0)
MFRC_PLAG  0.05  ! Fraction of Al2O3 going back to the particle (default: 0.0)
MFRC_PEUL1 1.0   ! Of Al2O3 going to smoke, fraction to type 1  (default: 0.0)
MFRC_PEUL2 1.0   ! Of Al2O3 going to smoke, fraction to type 2  (default: 0.0)
#

# RADIATION
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

! time-stepping control ------------------------------------------------------

# TIMESTEP
FLOWTYPE   1      ! 0=steady flow, 1=unsteady flow

! if FLOWTYPE=0
STARTITER     0   ! current iteration
MAXITER    20000  ! max. number of iterations
RESTOL     1.E-5  ! max. density residual to stop iterations
WRIITER    2000   ! offset between iterations to store solution
PRNITER    1      ! offset between iterations to print convergence
```

```
! if FLOWTYPE=1
TIMESTEP   1.0E-5 ! max. physical time step [s]
STARTTIME  0.0    ! current time
MAXTIME    6.0E-3 ! max. time simulated [s]
WRITIME    2.0E-3 ! time offset [s] to store solution
PRNTIME    1.0E-5 ! time offset [s] to print convergence
#

! numerics ------------------------------------------------------------------

# MULTIGRID
START    1       ! at which grid level to start (>0; 1=finest grid)
CYCLE    0       ! 0=no MG, 1=V-cycle, 2=W-cycle
REFINE   99999   ! no. of iterations before switching to next finer grid
#

# NUMERICS
BLOCK    0  0    ! applies to block ... (0 0 = to all)
CFL      7.5     ! CFL number
SMOOCF   1.0     ! coefficient of implicit residual smoothing (<0 - no smooth.)
DISCR    0       ! type of space discretization (0=central, 1=Roe, 2=MAPS)
K2       0.0     ! dissipation coefficient k2 (if discr=0)
1/K4     128.    ! dissipation coefficient 1/k4 (if discr=0)
ORDER    2       ! 1=first-order, 2=second-order, 4=fourth-order
LIMFAC   5.0     ! limiter coefficient (if discr=1)
ENTROPY  0.05    ! entropy correction coefficient (if discr=1)
#
```

5.4 ONERA C1 Numerical Experiment with Active Burning Particles

This example showcases how to activate coupling in specific regions and how to use the skewed clipped logarithmic distribution for the injection model. Activeness is only switched on for regions 1 through 41 and turned off for regions 42 through 52 (representing the nozzle region).

5.4.1 Input File

```
! Input file for C1 - viscous

! mapping of blocks to processors -------------------------------------------

# BLOCKMAP
NBLOCKS   0      ! no. of blocks per processor (0=automatic mapping)
#

! grid/solution format ------------------------------------------------------

# FORMATS
```

```
GRID      0      ! 0=Plot3D ASCII, 1=Plot3D binary, 2=HDF
SOLUTION  0      ! 0=ASCII, 1=binary, 2=HDF
#

! Random number generator-------------------------------------------------------

# RANDOM
SEED_OFFSET  0   ! Offset for seed of RNG (default = 0, otherwise: 1,2,3,etc)
#

! viscous/inviscid flow ---------------------------------------------------------

# FLOWMODEL
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL     1      ! 0=inviscid (Euler), 1=viscous (Navier-Stokes)
MOVEGRID  0      ! moving grid (0=no, 1=yes)
#

! reference values --------------------------------------------------------------

# REFERENCE
ABSVEL   1.0     ! reference velocity
DENS     1.0     ! reference density
CP       1004.5  ! specific heat coeff. at constant pressure [J/kgK]
GAMMA    1.4     ! ratio of specific heats
LENGTH   1.0     ! reference length
RENUM    5.0E04  ! reference Reynolds number
#

! probe -------------------------------------------------------------------------

# PROBE
NUMBER   0
#

! forces ------------------------------------------------------------------------

# FORCES
TYPE     1       ! 0=no forces calculated, 1=pressure forces, 2=1+viscous forces
#


! material definitions ----------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
```

```
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#

# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#

! multi-physics modules: ------------------------------------------------------

# TURBULENCE
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=laminar, 1=...
#

# SPECIES
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=perfect gas, 1=...
#

# CONPART
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=module not used (default: 1)
! the following quantities are default values for each CONPART_PTYPE below
DIAM   1.0E-6    ! diameter of an individual smoke particle
METH_VEL   0     ! (0=use fluid value, 1=eq eul)
INITC  1.E-9     ! initial concentration (overridden by input file)
1/K4   64.0      ! 1 / Artificial dissipation coefficient (k4)
NEGREPORT  0     ! (0=do not report on negative values,1=report) (default: 0)
#

# CONPART_PTYPE
MATERIAL     ALUMINUM_OXIDE ! material of which smoke consists
```

```
METH_VEL   1     ! (0=use fluid value, 1=eq eul)
DIAM   1.0E-6    ! diameter of an individual smoke particle
PUFF   1.0       ! puff factor: geometric volume / material volume (default: 1)
CLIPMODEL  1     ! (0=no clipping,1=clipping) (default: 0)
#

# CONPART_PTYPE
MATERIAL  OXIDIZER
INITC  0.01      ! initial concentration for oxidizer (overridden by input file)
CLIPMODEL  0     ! (0=no clipping,1=clipping) (default: 0)
#


# DISPART
BLOCK    0  0    ! applies to block ... (0 0 = to all)
USED     1       ! 0=module not used
NPCLSTOT        10000     ! Total Number of DisPart
EJECMODEL       1         ! Ejection Model
INJCVELRATIO    0.0       ! Injection Velocity Ratio
SPLOAD          5.00E+2   ! SuperParticle Loading
INJCBETA        5.00E+5   ! Injection beta Coefficient
INJCDIAMDIST    1         ! Injection Diameter Distribution Model
INJCDIAMMEAN    10.0E-06  ! Injection Mean Diameter
INJCDIAMMIN     5.0E-06   ! Injection Mean Diameter
INJCDIAMMAX     100.0E-06 ! Injection Mean Diameter
INJCSTDDEV      0.0       ! injection Standard Deviation
INTRPLMIXTMODEL 0         ! Interpolation Order for Mixture
NPCLSBUFFTOT    1000      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0         ! Breakup Model
BREAKUPFAC      2.0       ! Breakup Factor
BREAKUPWEBSWI   0         ! Breakup Weber Switch
#

# DISPART_NCONT
NCONT   2
ALUMINUM         0.1620  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.0180  ! MaterialName, injcMassRatio
#

# INRT_DEFAULT
BLOCK  1    41   ! applies to block ... (0 0 = to all)
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   1    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
PEUL1_ACTV  -1   ! (0=Passive, 1=Active) Activeness of Smoke type 1
PEUL2_ACTV  -1   ! (0=Passive, 1=Active) Activeness of Smoke type 2
#

# INRT_DEFAULT
BLOCK  42   52  ! applies to block ... (0 0 = to all)
MIXT_ACTV   1   ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   0   ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
```

```
PEUL1_ACTV  0   ! (0=Passive, 1=Active) Activeness of Smoke type 1
PEUL2_ACTV  0   ! (0=Passive, 1=Active) Activeness of Smoke type 2
#

# INRT_DRAG
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#

# INRT_SCOURING
BLOCK  1   41    ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
COEF1  0.25      ! Scouring Coefficient for Smoke type 1 (default: 1.0)
PLAG_ACTV  -1    ! Allow smoke to accumulate on particles
#

# INRT_SCOURING
BLOCK  42   52     ! applies to block ... (0 0 = to all)
USED   0         ! 0=interaction not used (default: 1)
COEF1  0.25      ! Scouring Coefficient for Smoke type 1 (default: 1.0)
PLAG_ACTV  -1    ! Allow smoke to accumulate on particles
#

# INRT_BURNING
BLOCK  1   41    ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MATERIAL_IN   ALUMINUM       ! material that burns
MATERIAL_OUT  ALUMINUM_OXIDE ! material created by the burning process
MATERIAL_OX   OXIDIZER       ! material used to oxidize
MODEL  1         ! (1=Beckstead correlation) (1 is default)
OX_USED    1     ! Whether to use oxidizer field (0=no,1=yes)  (default: 0)
VAPOR_METH 1     ! Model for vapor energy (0=do not use,1=use) (default: 0)
HEAT_COEF  1.0   ! Fraction of Actual Energy Released (default: 1.0)
MFRC_PLAG  0.1   ! Fraction of Al2O3 going back to the particle (default: 0.0)
MFRC_PEUL1 1.0   ! Of Al2O3 going to smoke, fraction to type 1  (default: 0.0)
#

# INRT_BURNING
BLOCK  42   52   ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MATERIAL_IN   ALUMINUM       ! material that burns
MATERIAL_OUT  ALUMINUM_OXIDE ! material created by the burning process
MATERIAL_OX   OXIDIZER       ! material used to oxidize
MODEL  1         ! (1=Beckstead correlation) (1 is default)
```

```
OX_USED    1     ! Whether to use oxidizer field (0=no,1=yes)  (default: 0)
VAPOR_METH 1     ! Model for vapor energy (0=do not use,1=use) (default: 0)
HEAT_COEF  1.0   ! Fraction of Actual Energy Released (default: 1.0)
MFRC_PLAG  0.1   ! Fraction of Al2O3 going back to the particle (default: 0.0)
MFRC_PEUL1 1.0   ! Of Al2O3 going to smoke, fraction to type 1  (default: 0.0)
#

# RADIATION
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

! time-stepping control -----------------------------------------------------

# TIMESTEP
FLOWTYPE   1      ! 0=steady flow, 1=unsteady flow

! if FLOWTYPE=0
STARTITER     0   ! current iteration
MAXITER    20000  ! max. number of iterations
RESTOL     1.E-5  ! max. density residual to stop iterations
WRIITER    2000   ! offset between iterations to store solution
PRNITER    1      ! offset between iterations to print convergence

! if FLOWTYPE=1
TIMESTEP   1.0E-5 ! max. physical time step [s]
STARTTIME  0.0    ! current time
MAXTIME    6.0E-3 ! max. time simulated [s]
WRITIME    2.0E-3 ! time offset [s] to store solution
PRNTIME    1.0E-5 ! time offset [s] to print convergence
#

! numerics ------------------------------------------------------------------

# MULTIGRID
START    1       ! at which grid level to start (>0; 1=finest grid)
CYCLE    0       ! 0=no MG, 1=V-cycle, 2=W-cycle
REFINE   99999   ! no. of iterations before switching to next finer grid
#

# NUMERICS
BLOCK    0  0    ! applies to block ... (0 0 = to all)
CFL      7.5     ! CFL number
SMOOCF   1.0     ! coefficient of implicit residual smoothing (<0 - no smooth.)
DISCR    0       ! type of space discretization (0=central, 1=Roe, 2=MAPS)
K2       0.0     ! dissipation coefficient k2 (if discr=0)
1/K4     128.    ! dissipation coefficient 1/k4 (if discr=0)
ORDER    2       ! 1=first-order, 2=second-order, 4=fourth-order
LIMFAC   5.0     ! limiter coefficient (if discr=1)
ENTROPY  0.05    ! entropy correction coefficient (if discr=1)
#
```

5.5 ONERA C1x Numerical Experiment with Active Burning Particles and Turbulence

This example showcases how to activate turbulence with Lagrangian particles.

5.5.1 Input File

```
! Input file for ONERA C1x - viscous with LES turbulence

! mapping of blocks to processors ------------------------------------------

# BLOCKMAP
NBLOCKS   0      ! no. of blocks per processor (0=automatic mapping)
#

! grid/solution format -----------------------------------------------------

# FORMATS
GRID      0      ! 0=Plot3D ASCII, 1=Plot3D binary, 2=HDF
SOLUTION  0      ! 0=ASCII, 1=binary, 2=HDF
#

! viscous/inviscid flow ----------------------------------------------------

# FLOWMODEL
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL     1      ! 0=inviscid (Euler), 1=viscous (Navier-Stokes)
MOVEGRID  0      ! moving grid (0=no, 1=yes)
#

! reference values ----------------------------------------------------------

# REFERENCE
ABSVEL   4.18E-3    ! 4.18E-3 absolute velocity [m/s]
PRESS    1.E+5   ! static pressure [Pa]
DENS     1.2     ! density [kg/m^3]
CP       1966.871025 ! specific heat coeff. at constant pressure [J/kgK]
GAMMA    1.210    ! ratio of specific heats
LENGTH   1.0     ! length [m]
RENUM    71.66   ! 71.66 Reynolds number (lam. viscosity = dens*absvel*length/renum)
PRLAM    0.468   ! laminar Prandtl number
PRTURB   0.9     ! turbulent Prandtl number
SCNLAM   0.22    ! laminar Schmidt number
SCNTURB  0.9     ! turbulent Schmidt number
#

! viscosity model -----------------------------------------------------------

# VISCMODEL
BLOCK  0  0       ! applies to block ... (0 0 = to all)
```

```
MODEL     1       ! 0=SutherLand, 1=Fixed, 2=Antibes
VISCOSITY 7.0E-05 ! reference viscosity
REFTEMP   110.0   ! reference temperature
SUTHCOEF  276.  ! 288.16 sutherland coefficient
#

! flow initialization ------------------------------------------------------

# INITFLOW
BLOCK     0  0   ! applies to block ... (0 0 = to all)
NDUMMY    3      ! no. of dummy cells
VELX      0.     ! velocity in x-direction [m/s]
VELY      0.     ! velocity in y-direction [m/s]
VELZ      0.     ! velocity in z-direction [m/s]
PRESS     1.5E+5 ! static pressure [Pa]
DENS      0.175496405    ! density [kg/m^3]
#

! probe ---------------------------------------------------------------------

# PROBE
NUMBER   8
12    1  14  12   ! block, icell, jcell, kcell (1=first physical cell)
17   12  27  12
18    6  27  12
18   36  27  12
19   30  27  12
20   23  27  12
21   17  27  12
22   25  27  12
#
WRITIME    3.65E-5    ! time offset [s] to store probe data
WRIITER    10       ! offset between iterations to store probe data
OPENCLOSE  1        ! open & close probe file every time (0=no, 1=yes)
#

! material definitions ------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
```

```
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#

# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#

! forces ---------------------------------------------------------------------

# FORCES
TYPE     1       ! 0=no forces calculated, 1=pressure forces, 2=1+viscous forces
#

! multi-physics modules: -----------------------------------------------------

# TURBULENCE
BLOCK  0  0        ! applies to block ... (0 0 = to all)
TURBMODEL  3       ! 0=laminar 1=FixedSmag 2=ScalSim (3)=DynSmag 4=DynMixed
OUTPUTNUMBER  2    !
CSMAGORINSKY  0.12 ! Model constant, only relevant for TURBMODEL=1
FILTERTYPE    0    ! 0=uniform, 1=non-uniform
DELTATYPE     0    ! 0=cuberoot-formula, 1=squareroot-formula
IFILTERWIDTH  2    ! filterwidth in I-direction/grid-spacing
JFILTERWIDTH  2    ! filterwidth in J-direction/grid-spacing
KFILTERWIDTH  2    ! filterwidth in K-direction/grid-spacing
IHOMOGENDIR   0    ! 0=non-homogeneous, 1=homogeneous I-direction
JHOMOGENDIR   0    ! 0=non-homogeneous, 1=homogeneous J-direction
KHOMOGENDIR   0    ! 0=non-homogeneous, 1=homogeneous K-direction
ENERGYMODEL   1    ! 0=OFF, 1=ACTIVE energy subgrid model
CALCVORTIC    1

! RANS
WALLDISTMETHOD  0
VISCFUNCTION    1
CDES            0.65
SMOOCF          0.0
DISCR           0    ! 0 central, 1 upwind
K2              0.0  ! (if DISCR=0)
```

```
1/K4            0.   ! (if DISCR=0)
ORDER           2    ! 1 1st, 2 2nd
#

# SPECIES
BLOCK  0  0      ! applies to block ... (0 0 = to all)
MODEL  0         ! 0=perfect gas, 1=...
#

# CONPART
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=module not used (default: 1)
! the following quantities are default values for each CONPART_PTYPE below
DIAM   1.0E-6    ! diameter of an individual smoke particle
METH_VEL   0     ! (0=use fluid value, 1=eq eul)
INITC  1.E-9     ! initial concentration (overridden by input file)
1/K4   64.0      ! 1 / Artificial dissipation coefficient (k4)
NEGREPORT  0     ! (0=do not report on negative values,1=report) (default: 0)
#

# CONPART_PTYPE
MATERIAL     ALUMINUM_OXIDE ! material of which smoke consists
METH_VEL   1     ! (0=use fluid value, 1=eq eul)
DIAM   1.0E-6    ! diameter of an individual smoke particle
PUFF   1.0       ! puff factor: geometric volume / material volume (default: 1)
CLIPMODEL  1     ! (0=no clipping,1=clipping) (default: 0)
#

# CONPART_PTYPE
MATERIAL  OXIDIZER
INITC  0.01      ! initial concentration for oxidizer (overridden by input file)
CLIPMODEL  0     ! (0=no clipping,1=clipping) (default: 0)
#

# DISPART
USED     1            ! 0=module not used
NPCLSTOT  20000        ! Total Number of DisPart
EJECMODEL    2        ! Ejection Model (1=Model1, 2=CRE)
INJCVELRATIO 0.01      ! Injection Velocity Ratio
SPLOAD       1.500E+4  ! SuperParticle Loading
INJCBETA     1.00E+0  ! injection beta Coefficient
INJCDIAMDIST 1        ! Injection Diameter Distribution Model
INJCDIAMMEAN  10.0E-06 ! Injection Mean Diameter
INJCDIAMMIN   10.0E-06 ! Injection Minimum Diameter
INJCDIAMMAX   10.0E-06 ! Injection Maximum Diameter
INJCSTDDEV      0.00   ! injection Standard Deviation
INTRPLMIXTMODEL 0      ! Interpolation Order for Mixture
NPCLSBUFFTOT    4000   ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0      ! Breakup Model
BREAKUPFAC      2.0    ! Breakup Factor
BREAKUPWEBSWI   0      ! Breakup Weber Switch
```

```
#

# DISPART_NCONT
NCONT   2
ALUMINUM         0.090  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.010  ! MaterialName, injcMassRatio
#

# RADIATION
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   0         ! 0=module not used
#

# INRT_DEFAULT
BLOCK  0    0    ! applies to block ... (0 0 = to all)
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   1    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
PEUL1_ACTV  -1   ! (0=Passive, 1=Active) Activeness of Smoke type 1
PEUL2_ACTV  -1   ! (0=Passive, 1=Active) Activeness of Smoke type 2
#

# INRT_DRAG
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
BLOCK  0  0      ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#

# INRT_SCOURING
BLOCK  0   0     ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
COEF1  0.25      ! Scouring Coefficient for Smoke type 1 (default: 1.0)
PLAG_ACTV  -1    ! Allow smoke to accumulate on particles
#

# INRT_BURNING
BLOCK  0   0     ! applies to block ... (0 0 = to all)
USED   1         ! 0=interaction not used (default: 1)
MATERIAL_IN   ALUMINUM       ! material that burns
MATERIAL_OUT  ALUMINUM_OXIDE ! material created by the burning process
MATERIAL_OX   OXIDIZER       ! material used to oxidize
MODEL  1         ! (1=Beckstead correlation) (1 is default)
OX_USED    1     ! Whether to use oxidizer field (0=no,1=yes)  (default: 0)
VAPOR_METH 1     ! Model for vapor energy (0=do not use,1=use) (default: 0)
HEAT_COEF  1.0   ! Fraction of Actual Energy Released (default: 1.0)
MFRC_PLAG  0.1   ! Fraction of Al2O3 going back to the particle (default: 0.0)
```

```
MFRC_PEUL1 1.0   ! Of Al2O3 going to smoke, fraction to type 1  (default: 0.0)
#

! time-stepping control ---------------------------------------------------

# TIMESTEP
FLOWTYPE   1      ! 0=steady flow, 1=unsteady flow

! if FLOWTYPE=0
STARTITER     0   ! current iteration
MAXITER    20000  ! max. number of iterations
RESTOL     1.E-5  ! max. density residual to stop iterations
WRIITER    2000   ! offset between iterations to store solution
PRNITER    1      ! offset between iterations to print convergence

! if FLOWTYPE=1
TIMESTEP   5.0E-07 ! max. physical time step [s]
STARTTIME  2.6E-02  ! current time
MAXTIME    2.8E-02 ! max. time simulated [s]
WRITIME    1.0E-03 ! time offset [s] to store solution
PRNTIME    0.0     ! time offset [s] to print convergence
#

! time averaged statistics for unsteady flow -------------------------------

# STATISTICS
DOSTAT     0     ! 1=ON, 0=OFF
RESTART    0     ! restart switch: 1 = continued process, 0 = new process
MIXTNSTAT  11    ! number of mixture statistics with their ID's below
MIXTSTATID 01 02 03 04 06 11 22 33 44 23 66
                 ! 1=rho 2=u 3=v 4=w 5=T 6=p 7=vsound 8=muel 9=tcol 22=uu etc
TURBNSTAT  2     ! number of mixture statistics with their ID's below
TURBSTATID 01 03
                 ! 1=muet 2=tcot 3=cdyn 4:7=t11,t22,t33,t12 8=mmij 9=mlij
#

! numerics -----------------------------------------------------------------

# MULTIGRID
START    1       ! at which grid level to start (>0; 1=finest grid)
CYCLE    0       ! 0=no MG, 1=V-cycle, 2=W-cycle
REFINE   99999   ! no. of iterations before switching to next finer grid
#

# NUMERICS
BLOCK    0  0    ! applies to block ... (0 0 = to all)
CFL      3.0     ! CFL number
SMOOCF   0.70    ! coefficient of implicit residual smoothing (<0 - no smooth.)
DISCR    0       ! type of space discretization (0=central, 1=Roe, 2=MAPS)
K2       0.0     ! dissipation coefficient k2 (if discr=0)
1/K4     1024.    ! dissipation coefficient 1/k4 (if discr=0)
```

```
ORDER    2       ! 1=first-order, 2=second-order, 4=fourth-order
LIMFAC   5.0     ! limiter coefficient (if discr=1)
ENTROPY  0.05    ! entropy correction coefficient (if discr=1)
#

! post processing ----------------------------------------------------------

# POST
PLTTYPE   2
TIME      8.05058E-02
ITER      0
OUTFORMAT 3
TURBFLAG  1
#
```

Chapter 6

Examples and Test Problems for Rocflu

This chapter provides several test case examples to run Rocflu with Lagrangian particles under distinct modes of operations. Test cases based on single region are outlined.

6.1 Cubes to generate set positions of particles

This example provides the procedure to set particles with initial positions.

6.1.1 Input File

```
# FORMATS
GRID      0     ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
SOLUTION  0 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
GRIDSRC   0 ! 0 - CENTAUR ASCII, 1 - VGRIDNS, 2 - MESH3D
#

# FLOWMODEL
MODEL    0  ! 0 - Euler, 1 - Navier-Stokes
MOVEGRID 0 ! 0 - static grid, 1 - moving grid
#

# NUMERICS
CFL      3.0 ! CFL number
DISCR    1      ! Type of space discretization (1 - Roe, 2 - MAPS)
ORDER    1      ! Order of accuracy (1 - first, 2 - second)
ENTROPY  0.05   ! Entropy correction coefficient (if DISCR=1)
#

# TIMESTEP
FLOWTYPE   1     ! 0 - steady flow, 1 - unsteady flow
TIMESTEP   1.00E-07 ! max. physical time step [s]
STARTTIME  0.0      ! current time
MAXTIME    1.00E-06 ! max. time simulated [s]
WRITIME    0.1      ! time offset [s] to store solution
PRNTIME    1.0E-06  ! time offset [s] to print convergence
#
```

```
# REFERENCE
GAMMA 1.4
CP 1004.64
DENS    1.15629693398
ABSVEL 101.179354922
LENGTH  10.0
RENUM   1000.0
#

# PROBE
NUMBER 0
#
#

# VISCMODEL
MODEL     1       ! 0=SutherLand, 1=Fixed, 2=Antibes
VISCOSITY 3.6E-04 ! reference viscosity
REFTEMP   110.0   ! reference temperature
SUTHCOEF  274.4290599  ! sutherland coefficient
#

# INITFLOW
FLAG    1
DENS 1.0
VELX 0.0
VELY 0.0
VELZ  0.0
PRESS 1.0E+05
#

# POST
SPECFLAG 1
#

! material definitions ------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS 0.70    ! surface tension
#

! multi-physics modules: ----------------------------------------------------

# DISPART
USED     1             ! 0=module not used
NPCLSTOT     100000    ! Total Number of DisPart
```

```
INJCMODEL     1        ! Injection Model
INJCVELRATIO  0.0      ! Injection Velocity Ratio
SPLOAD        1.00     ! SuperParticle Loading
INJCDIAMMEAN  10.0E-06 ! Injection Mean Diameter
INJCDIAMMIN    6.0E-06 ! Injection Minimum Diameter
INJCDIAMMAX  100.0E-06 ! Injection Maximum Diameter
INJCSTDDEV     0.00    ! injection Standard Deviation
INJCTIMECOEFF  5.00E+5 ! injection Time Coefficient
INTRPLMIXTMODEL 0      ! Interpolation Order for Mixture
NPCLSBUFFTOT   10      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0      ! Breakup Model
BREAKUPFAC      2.0    ! Breakup Factor
BREAKUPWEBSWI   0      ! Breakup Weber Switch
FINDPCLMETHOD   1      ! 1:Trajectory, 2: Brute Force, 3: Octree, 4:Known Vicinity
#

# DISPART_NCONT
NCONT   1
ALUMINUM         0.20  ! MaterialName, injcMassRatio
#

# DISPART_INIT
FLAG 1           ! 1: Scratch, 4: Random State
NPCLSRAND 0      ! Number of initial random particles
#
NUMBER 5
0.01 0.02 0.03 10.0E-06 3000.0 1.0 ! posX, posY, posZ, diam, temp, spLoad
0.10 0.10 0.10 20.0E-06 3100.0 1.0 ! posX, posY, posZ, diam, temp, spLoad
0.11 0.15 0.15 50.0E-06 3500.0 1.0 ! posX, posY, posZ, diam, temp, spLoad
0.12 0.15 0.15  5.0E-06 3000.0 1.0 ! posX, posY, posZ, diam, temp, spLoad
0.14 0.20 0.20 25.0E-06 3200.0 1.0 ! posX, posY, posZ, diam, temp, spLoad
#

# INRT_DEFAULT
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   0    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
#

# INRT_DRAG
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#
```

6.2 Cubes to generate random positions of particles

This example provides the procedure to

6.2.1 Input File

```
# FORMATS
GRID      0     ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
SOLUTION  0 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
GRIDSRC   0 ! 0 - CENTAUR ASCII, 1 - VGRIDNS, 2 - MESH3D
#

# FLOWMODEL
MODEL    0  ! 0 - Euler, 1 - Navier-Stokes
MOVEGRID 0 ! 0 - static grid, 1 - moving grid
#

# NUMERICS
CFL      3.0 ! CFL number
DISCR    1      ! Type of space discretization (1 - Roe, 2 - MAPS)
ORDER    1      ! Order of accuracy (1 - first, 2 - second)
ENTROPY  0.05   ! Entropy correction coefficient (if DISCR=1)
#

# TIMESTEP
FLOWTYPE   1     ! 0 - steady flow, 1 - unsteady flow
TIMESTEP   1.00E-07 ! max. physical time step [s]
STARTTIME  0.0      ! current time
MAXTIME    1.00E-06 ! max. time simulated [s]
WRITIME    0.1      ! time offset [s] to store solution
PRNTIME    1.0E-06  ! time offset [s] to print convergence
#

# REFERENCE
GAMMA 1.4
CP 1004.64
DENS    1.15629693398
ABSVEL 101.179354922
LENGTH  10.0
RENUM   1000.0
#

# PROBE
NUMBER 0
#
#

# VISCMODEL
MODEL     1       ! 0=SutherLand, 1=Fixed, 2=Antibes
VISCOSITY 3.6E-04 ! reference viscosity
REFTEMP   110.0   ! reference temperature
```

```
SUTHCOEF  274.4290599  ! sutherland coefficient
#

# INITFLOW
FLAG    1
DENS 1.0
VELX 0.0
VELY 0.0
VELZ  0.0
PRESS 1.0E+05
#

# POST
SPECFLAG 1
#

! material definitions --------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS 0.70    ! surface tension
#

! multi-physics modules: -------------------------------------------------------

# DISPART
USED     1             ! 0=module not used
NPCLSTOT     100000    ! Total Number of DisPart
INJCMODEL     1        ! Injection Model
INJCVELRATIO  0.0      ! Injection Velocity Ratio
SPLOAD        1.00     ! SuperParticle Loading
INJCDIAMMEAN  10.0E-06 ! Injection Mean Diameter
INJCDIAMMIN    6.0E-06 ! Injection Minimum Diameter
INJCDIAMMAX  100.0E-06 ! Injection Maximum Diameter
INJCSTDDEV     0.00    ! injection Standard Deviation
INJCTIMECOEFF  5.00E+5 ! injection Time Coefficient
INTRPLMIXTMODEL 0      ! Interpolation Order for Mixture
NPCLSBUFFTOT   10      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0      ! Breakup Model
BREAKUPFAC      2.0    ! Breakup Factor
BREAKUPWEBSWI   0      ! Breakup Weber Switch
FINDPCLMETHOD   1      ! 1:Trajectory, 2: Brute Force, 3: Octree, 4:Known Vicinity
#

# DISPART_NCONT
NCONT   1
ALUMINUM         0.20  ! MaterialName, injcMassRatio
```

```
#

# DISPART_INIT
FLAG 4           ! 1: Scratch, 4: Random State
NPCLSRAND 10000  ! Number of initial random particles
#
NUMBER 2
5.0E-06  3000.0 1.0  ! diamMin, tempMin, spLoadMin
20.0E-06 4000.0 1.0  ! diamMax, tempMax, spLoadMax
#

# INRT_DEFAULT
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   0    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
#

# INRT_DRAG
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#
```

6.3 ONERA C0 Numerical Experiment with Passive Particles

The ONERA C0 example is described in various papers and consists of an injecting bottom wall, a top symmetry plane, an exit plane and a non-slip wall.

6.3.1 Input File

```
# FORMATS
GRID      1 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
SOLUTION  0 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
GRIDSRC   0 ! 0 - CENTAUR ASCII, 1 - VGRIDNS, 2 - MESH3D
#

# FLOWMODEL
MODEL    0  ! 0 - Euler, 1 - Navier-Stokes
MOVEGRID 0 ! 0 - static grid, 1 - moving grid
#

# NUMERICS
CFL      5.0 ! CFL number
DISCR    1      ! Type of space discretization (1 - Roe, 2 - MAPS)
ORDER    2      ! Order of accuracy (1 - first, 2 - second)
ENTROPY  0.05   ! Entropy correction coefficient (if DISCR=1)
DISSFACT 1.00   ! Dissipation factor for Roe scheme
```

```
#

# TIMESTEP
FLOWTYPE  1     ! 0 - steady flow, 1 - unsteady flow
TIMESTEP   2.0E-07  ! max. physical time step [s]
STARTTIME  0.0E-03  ! current time
MAXTIME    4.0E-07  ! max. time simulated [s]
WRITIME    4.0E-07  ! time offset [s] to store solution
PRNTIME    0.0      ! time offset [s] to print convergence
RKSCHEME   2        ! 1 - classical RK4, 2 - low-storage Wray RK3
#

# REFERENCE
CP       1003.45  ! specific heat coeff. at constant pressure [J/kgK]
GAMMA    1.4      ! ratio of specific heats
#

# FORCES
TYPE      1  ! 0 - no, 1 - pressure, 2 - pressure and viscous forces
#

# VISCMODEL
MODEL     1       ! 0=SutherLand, 1=Fixed, 2=Antibes
VISCOSITY 3.6E-04 ! reference viscosity
REFTEMP   110.0   ! reference temperature
SUTHCOEF  288.16  ! sutherland coefficient
#

# PROBE
NUMBER 2
0.0001  0.01 -0.005
0.58099 0.01 -0.005
#
WRITIME 1.E-5
OPENCLOSE 1
#

# INITFLOW
FLAG    1
DENS 1.0
VELX 0.0
VELY 0.0
VELZ  0.0
PRESS   1.5E+5
#

# POST
PLTTYPE    2
PLTVOLFLAG 1
MERGEFLAG  0
SPECFLAG   1
```

```
#

! material definitions ------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#

# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#

! multi-physics modules: -----------------------------------------------------

# SPECIES
USED 0
NSPECIES 0
#

# DISPART
USED     1             ! 0=module not used
NPCLSTOT   2000        ! Total Number of DisPart
EJECMODEL    2         ! Ejection Model (1=Model1, 2=CRE)
INJCVELRATIO 0.0       ! Injection Velocity Ratio
SPLOAD       2.50E+3   ! SuperParticle Loading
INJCBETA     1.00E+0   ! injection beta Coefficient
```

```
INJCDIAMDIST 1         ! Injection Diameter Distribution Model
INJCDIAMMEAN   1.0E-05 ! Injection Mean Diameter
INJCDIAMMIN    1.0E-05 ! Injection Minimum Diameter
INJCDIAMMAX    1.0E-05 ! Injection Maximum Diameter
INJCSTDDEV     0.00    ! injection Standard Deviation
INTRPLMIXTMODEL 0      ! Interpolation Order for Mixture
NPCLSBUFFTOT 1000      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0      ! Breakup Model
BREAKUPFAC      2.0    ! Breakup Factor
BREAKUPWEBSWI   0      ! Breakup Weber Switch
FINDPCLMETHOD   1      ! Method to Track Particles (1: Traj, 2: Brute, 3: OctTree, 4: Known-Vicinity)
#

# DISPART_NCONT
NCONT   1
ALUMINUM         0.20  ! MaterialName, injcMassRatio
#

# DISPART_INIT
FLAG 1           ! 1: Scratch, 4: Random State
NPCLSRAND 0      ! Number of initial random particles
#
NUMBER 0
#

# INRT_DEFAULT
2D_AVERAGE  0         ! (0 = Do not Average, 1=average in k-direction)
MIXT_ACTV   1         ! (0=Ghost, 1=Real) Default Tag for Gas (1=Real is default)
PLAG_ACTV   0         ! (0=Ghost, 1=Real) Default Tag for Lagrangian Particles
#

# INRT_DRAG
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#
```

6.3.2 Boundary Condition `.bc` File

```
# BC_SLIPW
PATCH   1 1
NAME    HeadEndWall
#

# BC_INJECT
PATCH           2 2
```

```
NAME            Injection
DISTRIB         0
MFRATE          2.42   ! mass flow rate [kg/(m^2*s)] (if distrib=0)
TEMP            303.   ! injection temperature [K] (if distrib=0)21.20
RFVFU           0.0
RFVFV           0.0
RFVFW           0.0
#

# BC_OUTFLOW
PATCH           3 3
NAME            Outflow
DISTRIB         0
TYPE            1
PRESS           1.5E+05
#

# BC_SLIPW
PATCH   4 4
NAME    TopSymmetry
#

# BC_SLIPW
PATCH   5 6
NAME    SideSymmetry
#

# END
```

6.4 ONERA C1 Numerical Experiment with Active Burning Particles

6.4.1 Input File

```
# FORMATS
GRID      1 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
SOLUTION  0 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
GRIDSRC  10 ! 0 - CENTAUR ASCII, 1 - VGRIDNS, 2 - MESH3D
#

# FLOWMODEL
MODEL    0  ! 0 - Euler, 1 - Navier-Stokes
MOVEGRID 0 ! 0 - static grid, 1 - moving grid
#

# NUMERICS
CFL      5.0 ! CFL number
DISCR    1      ! Type of space discretization (1 - Roe, 2 - MAPS)
ORDER    2      ! Order of accuracy (1 - first, 2 - second)
ENTROPY  0.05   ! Entropy correction coefficient (if DISCR=1)
```

```
DISSFACT 0.10   ! Dissipation factor for Roe scheme
#

# TIMESTEP
FLOWTYPE  1 ! 0 - steady flow, 1 - unsteady flow
TIMESTEP   2.00E-07 ! max. physical time step [s]
STARTTIME  0.0E+00 ! current time
MAXTIME    1.0E-02 ! max. time simulated [s]
WRITIME    1.0E-03 ! time offset [s] to store solution
PRNTIME    0.0     ! time offset [s] to print convergence
RKSCHEME   2       ! Timestepping Scheme (1: RK-4 Classical, 2: Low Storage RK-3)
#

# REFERENCE
CP       2439.04 ! specific heat coeff. at constant pressure [J/kgK]
GAMMA    1.14    ! ratio of specific heats
#

# FORCES
TYPE      1  ! 0 - no, 1 - pressure, 2 - pressure and viscous forces
#

# VISCMODEL
MODEL     1       ! 0=SutherLand, 1=Fixed, 2=Antibes
VISCOSITY 3.6E-04 ! reference viscosity
REFTEMP   110.0   ! reference temperature
SUTHCOEF  288.16  ! sutherland coefficient
#

# PROBE
NUMBER 2
0.0001 0.045 0.005
0.4699 0.045 0.005
#
WRITIME 1.E-5
OPENCLOSE 1
#

# INITFLOW
FLAG    1
DENS 1.0
VELX 0.0
VELY 0.0
VELZ  0.0
PRESS 1.5E+5
#

# POST
PLTTYPE    2
PLTVOLFLAG 1
MERGEFLAG  0
```

```
#

# TRANSFORM
FLAG    1
SCALE_X 0.470000
SCALE_Y 0.470000
SCALE_Z 1.000000
ANGLE_X 0.000000
ANGLE_Y 0.000000
ANGLE_Z 0.000000
#
! material definitions ------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#

# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#

! multi-physics modules: -----------------------------------------------------

# SPECIES
USED 1
NSPECIES 2
```

```
#

# SPECIES_TYPE
MATERIAL   ALUMINUM_OXIDE
FROZENFLAG 0
INITVAL    1.E-9
SCHMIDTNO  1.0
SOURCETYPE 0
#

# SPECIES_TYPE
MATERIAL   OXIDIZER
FROZENFLAG 0
INITVAL    0.01
SCHMIDTNO  1.0
SOURCETYPE 0
#

# DISPART
USED     1            ! 0=module not used
NPCLSTOT  10000        ! Total Number of DisPart
EJECMODEL    2        ! Ejection Model (1=Model1, 2=CRE)
INJCVELRATIO 0.0      ! Injection Velocity Ratio
SPLOAD       1.00E+1  ! SuperParticle Loading
INJCBETA     1.00E+0  ! injection beta Coefficient
INJCDIAMDIST 2        ! Injection Diameter Distribution Model
INJCDIAMMEAN  30.0E-06 ! Injection Mean Diameter
INJCDIAMMIN    5.0E-06 ! Injection Minimum Diameter
INJCDIAMMAX  240.0E-06 ! Injection Maximum Diameter
INJCSTDDEV     1.30    ! injection Standard Deviation
INTRPLMIXTMODEL 0     ! Interpolation Order for Mixture
NPCLSBUFFTOT 1000      ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0      ! Breakup Model
BREAKUPFAC      2.0    ! Breakup Factor
BREAKUPWEBSWI   0      ! Breakup Weber Switch
FINDPCLMETHOD   1      ! Particle Tracking Method (1: Trajectory, 2: Brute, 3: Octree, 4: Vicinity)
#

# DISPART_NCONT
NCONT   2
ALUMINUM         0.162  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.010  ! MaterialName, injcMassRatio
#

# DISPART_INIT
FLAG 1
#
NUMBER 0
#

# INRT_DEFAULT
```

```
2D_AVERAGE  0    ! (0 = Do not Average, 1=average in k-direction)
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   1    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
SPEC1_ACTV -1    ! (0=Passive, 1=Active) Activeness of Smoke type 1
SPEC2_ACTV -1    ! (0=Passive, 1=Active) Activeness of Smoke type 2
#

# INRT_DRAG
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
#

# INRT_SCOURING
USED   1         ! 0=interaction not used (default: 1)
COEF1  0.25      ! Scouring Coefficient for Smoke type 1 (default: 1.0)
PLAG_ACTV  -1    ! Allow smoke to accumulate on particles
#

# INRT_BURNING
USED   1         ! 0=interaction not used (default: 1)
MATERIAL_IN   ALUMINUM       ! material that burns
MATERIAL_OUT  ALUMINUM_OXIDE ! material created by the burning process
MATERIAL_OX   OXIDIZER       ! material used to oxidize
MODEL  1         ! (1=Beckstead correlation) (1 is default)
OX_USED    1     ! Whether to use oxidizer field (0=no,1=yes)  (default: 0)
VAPOR_METH 1     ! Model for vapor energy (0=do not use,1=use) (default: 0)
HEAT_COEF  1.0   ! Fraction of Actual Energy Released (default: 1.0)
MFRC_PLAG  0.1   ! Fraction of Al2O3 going back to the particle (default: 0.0)
MFRC_SPEC1 1.0   ! Of Al2O3 going to smoke, fraction to type 1  (default: 0.0)
#
```

6.4.2 Boundary Condition `.bc` File

```
# BC_NOSLIP
PATCH   1 1
NAME    SolidWall
ADIABAT 1
#

# BC_INJECT
PATCH           2 2
NAME            InjectionWall
MFRATE          21.201
TEMP            3387.0
RFVFU           0.0
```

```
RFVFV           0.0
RFVFW           0.0
SPEC1           1.E-3  ! AlOx     mfrate = 1.E-3*21.201
SPEC2           0.18   ! Oxidizer mfrate = 0.18 *21.201
#

# BC_NOSLIP
PATCH   3 3
NAME    SolidWall
ADIABAT 1
#

# BC_OUTFLOW
PATCH           4 4
TYPE            0
PRESS           1.0E+5
#

# BC_SLIPW
PATCH   5 7
NAME    SlipWall
#

# END
```

6.5 LP6 Numerical Experiment with Passive non-Burning Particles

This example showcases how to activate coupling in specific regions and how to use the skewed clipped logarithmic distribution for the injection model.

6.5.1 Input File

```
# FORMATS
GRID      0 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
SOLUTION  0 ! 0 - ROCFLU ASCII, 1 - ROCFLU binary, 2 - ROCFLU HDF
GRIDSRC   0 ! 0 - CENTAUR ASCII, 1 - VGRIDNS, 2 - MESH3D
#

# FLOWMODEL
MODEL    1  ! 0 - Euler, 1 - Navier-Stokes
MOVEGRID 0 ! 0 - static grid, 1 - moving grid
#

# NUMERICS
CFL      2.0    ! CFL number
DISCR    1      ! Type of space discretization (1 - Roe, 2 - MAPS)
ORDER    2      ! Order of accuracy (1 - first, 2 - second)
ENTROPY  0.05   ! Entropy correction coefficient (if DISCR=1)
```

```
DISSFACT 0.10   ! Dissipation factor for Roe scheme
#

# TIMESTEP
FLOWTYPE  1      ! 0 - steady flow, 1 - unsteady flow
TIMESTEP  4.0E-7 ! Max. physical time step
STARTTIME 0.0    ! Current iteration
MAXTIME   5.0E-2 ! Maximum number of iterations
WRITIME   1.0E-3 ! Offset between iterations to store solutions
PRNTIME   0.0    ! Offset between iterations to print convergence
RKSCHEME  2      ! 1=RK4; 2=RK3
#

# PROBE
NUMBER 2
0.0001 0.0  0.0
0.3999 0.0  0.0
#
WRITIME 1.E-5
OPENCLOSE 1
#

# REFERENCE
CP      1006.0  ! Specific heat coeff. at constant pressure (J/kgK)
GAMMA   1.4     ! Ratio of specific heats
PRLAM   0.71    ! Laminar Prandtl number
#

# FORCES
TYPE      1     ! 0 - no, 1 - pressure, 2 - pressure and viscous forces
#

# VISCMODEL
MODEL     1          ! 0=SutherLand, 1=Fixed, 2=Antibes
VISCOSITY 1.7894E-5  ! reference viscosity
REFTEMP   110.0      ! reference temperature
SUTHCOEF  288.16     ! sutherland coefficient
#

# INITFLOW
FLAG    1
DENS    1.220745701
VELX    0.0
VELY    0.0
VELZ    0.0
PRESS   1.0E+5
#

# POST
INTERTYPE  0
PLTTYPE    2
```

```
PLTVOLFLAG 1
MERGEFLAG  0
#

! material definitions ------------------------------------------------------

# MATERIAL
NAME   ALUMINUM
PHASE  LIQUID
MOLW   0.0269815 ! molecular weight (in SI units)
DENS   1766.0    ! density
SPHT   1375.0    ! specific heat
SURFTENS  0.85   ! surface tension
TBOIL  3000.0    ! boiling point
TMELT   933.5    ! melting point
#

# MATERIAL
NAME   ALUMINUM_OXIDE
PHASE  LIQUID
MOLW   0.101961  ! molecular weight (in SI units)
DENS   1600.0    ! density
SPHT   1100.0    ! specific heat
SURFTENS  0.69   ! surface tension
TBOIL  4000.0    ! boiling point
TMELT  2054.0    ! melting point
#

# MATERIAL
NAME   OXIDIZER
PHASE  GAS
MOLW   1.0  ! molecular weight (in SI units)
DENS   1.0  ! density
SPHT   1.0  ! specific heat
SURFTENS 1.0    ! surface tension
TBOIL  1000.0   ! boiling point
TMELT  1000.0   ! melting point
#

! multi-physics modules: -----------------------------------------------------

# TURBULENCE
MODEL  0         ! 0=laminar, 1=...
#

# SPECIES
MODEL  0         ! 0=perfect gas, 1=...
#

# RADIATION
USED   0         ! 0=module not used
```

```
#

# CONPART
USED   0         ! 0=module not used (default: 1)
#

# DISPART
USED     1             ! 0=module not used
NPCLSTOT    10000      ! Total Number of DisPart
EJECMODEL    2         ! Ejection Model (1=Model1, 2=CRE)
INJCVELRATIO 0.0       ! Injection Velocity Ratio
SPLOAD       2.00E+1   ! SuperParticle Loading
INJCBETA     1.00E+0   ! injection beta Coefficient
INJCDIAMDIST 2         ! Injection Diameter Distribution Model
INJCDIAMMEAN  30.0E-06 ! Injection Mean Diameter
INJCDIAMMIN    5.0E-06 ! Injection Minimum Diameter
INJCDIAMMAX  240.0E-06 ! Injection Maximum Diameter
INJCSTDDEV     1.30    ! Injection Standard Deviation
INTRPLMIXTMODEL 0      ! Interpolation Order for Mixture
NPCLSBUFFTOT   2000    ! Total Size of Communication Buffer for DisPart
BREAKUPMODEL    0      ! Breakup Model
BREAKUPFAC      2.0    ! Breakup Factor
BREAKUPWEBSWI   0      ! Breakup Weber Switch
#

# DISPART_NCONT
NCONT   2
ALUMINUM         0.180  ! MaterialName, injcMassRatio
ALUMINUM_OXIDE   0.020  ! MaterialName, injcMassRatio
#

# DISPART_INIT
FLAG 1           ! 1: Scratch, 4: Random State
NPCLSRAND 0      ! Number of initial random particles
#
NUMBER 0
#

# INRT_DEFAULT
MIXT_ACTV   1    ! (0=Passive, 1=Active) Activeness of Gas
PLAG_ACTV   0    ! (0=Passive, 1=Active) Activeness of Lagrangian Particles
#

# INRT_DRAG
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Schiller-Naumann correlation) (2 is default)
#

# INRT_HEAT_TRANSFER_NONBURN
USED   1         ! 0=interaction not used (default: 1)
MODEL  2         ! (1=Stokes, 2=Ranz-Marshall correlation) (2 is default)
```

```
#
```

6.5.2 Boundary Condition .bc File

```
# BC_INJECT
PATCH   1 1
NAME    InjectionWall
MFRATE  55.25
TEMP    288.15
RFVFU   0.0
RFVFV   0.0
RFVFW   0.0
#

# BC_SLIPW
PATCH   2 2
NAME    NozzleNose
#

# BC_SLIPW
PATCH   3 3
NAME    Bucket
#

# BC_SLIPW
PATCH   4 4
NAME    NozzleWalls
#

# BC_OUTFLOW
PATCH   5 5
NAME    Outflow
TYPE    1
PRESS   1.0E+4
#

# BC_SLIPW
PATCH   6 6
NAME    Inhibitors
#

# BC_SLIPW
PATCH   7 7
NAME    HeadEnd
#

# BC_SLIPW
PATCH   8 9
NAME    SideWalls
#
```

```
# END
```