**Title**

# PROLOG V3.2

# Application Manual

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# PROLOG V3.2 – Application Manual

This Manual contains task-oriented instructions that show you how to use the PROLOG module.

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# 1 REFERENCE DOCUMENTS

[RD1] "PLUME V3.2 – Interface files definition". P. Chèoux-Damas. Doc. MMS : S413/RT/41.97. 24/10/97.

[RD2] "PLUMFLOW V3.2 procedure – Application manual". C. Theroude, P. Chèoux-Damas. Doc. Astrium : MOS.NT.CT.3682776.02

## 2 INTRODUCTION

The PROLOG module is an extension of the PLUMFLOW software for the computation of the thruster flow field. The objective of PROLOG is to compute the flow field extension, far from the thruster in the front-flow, as well as in the backflow, adapted for each type of the flow regime: continuum, free molecular and transition regimes. The module provides the results for the mean flow field as well as for multi-species flow field.

The computation of the PROLOG module is divided into three steps depending on the three flow regimes mentioned before. The continuum extension consists of an isentropic expansion of the gas with the conservation of the mass flow rate along the streamlines. The free molecular regime is computed using a ray-tracing method. The transition regime is then computed with an interpolation between the continuum and the free molecular flow field.

The PROLOG module is integrated inside the PLUMFLOW software and is interfaced with the ODE, CEC, NAVIER, MCLIP and TRAJET modules.

This document is the application manual of the PROLOG module. Chapter 3 presents the PROLOG module. Chapter 4 is dedicated to an exhaustive description of the input and output files of the module. Chapter 5 gives an example of the use of the module, with some advises to the user. Chapter 6 presents the theoretical description of the PROLOG modelling approach.

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## 3 PROLOG DESCRIPTION

### 3.1 FUNCTIONAL DESCRIPTION

The PROLOG computer program is used to extend the gas flow from the NAVIER or MCLIP computation domain to the 'infinity' and taking into account the different flow regimes.

The objective of the PROLOG module is:

**According to:**

- The thermodynamic properties of the gas,

- The gas species properties,

- The results of NAVIER or MCLIP computation,

- The dimensions of the region to be computed.

**Computes:**

- The flow field parameters for the continuum regime for the mean flow and for each species of the gas,

- The flow field parameters for the free molecular regime for the mean flow and for each species of the gas,

- The flow field parameters for the transition regime for the mean flow and for each species of the gas.

### 3.2 METHOD OF ANALYSIS

This paragraph presents the method of analysis for the PROLOG computation. For more details, see the theoretical aspects in chapter 6. The computation of the PROLOG extension is divided into three steps, computing each flow regime:

**Continuum regime expansion:**

The continuum flow regime is calculated in a streamlines-based mesh and is extended along the streamlines using a source-point method and assuming isentropic expansion. The computation of the flow field parameters assumes mass flow rate conservation along the streamlines.

**Free molecular regime expansion:**

The free molecular flow regime is computed using a particle approach, a Monte-Carlo – ray-tracing method, where a representative sample of molecules is propagated in the whole computing domain from the limit of the continuum domain called the freezing surface. The macroscopic flow parameters are calculated by meaning the ray contribution of the flow parameters in each cell of the mesh.

**Bridging:**

The bridging provides the flow field result in the whole computation domain with respect of each flow regime. It computes the transition flow regime using a linear interpolation between the continuum flow regime and the free molecular flow regime.

## 3.3 SOFTWARE LIMITATIONS

In the continuum flow regime computation, the area of the initial flow field domain must be large enough to fit with the hypothesis of a source-flow at the boundary.

## 4    PROLOG INPUT/OUTPUT

### 4.1    PROLOG ARCHITECTURE

The PROLOG module is composed of three main subroutines that must be executed consecutively:

- CONTINUE computes the continuum flow regime.

- FREEMOL computes the free molecular flow regime.

- BRIDGING computes the bridging between the continuum flow and the free molecular flow regimes.

The PROLOG input files are:

| File | Function |
|---|---|
| "thruster name".THERMO | Gas table giving versus the temperature : $H, W_{mol}, \gamma, T, P, C_{p}, \mu, Pr$. |
| "thruster name".T07 | Gas group of species properties generated by ODE or CEC |
| "thruster name".FLOW | Flow-field file data generated by NAVIER or MCLIP |
| "thruster name".PRI | User input file of the run parameters |

The PROLOG output files are:

| File | Function |
|---|---|
| "thruster name"C.FLOW | Flow-field parameters for continuum flow regime and nozzle geometry. |
| "thruster name"FC.FLOW | Flow-field parameters for free molecular flow regime in Cartesian mesh for the sub-domain specified by the user and freezing surface geometry. |
| "thruster name"FS.FLOW | Flow-field parameters for free molecular flow regime in streamlines-based mesh and freezing surface geometry. |
| "thruster name"B.FLOW | Flow-field parameters for the bridging flow and freezing surface geometry. |
| "thruster name".PRO | Output listing file summarizing the run parameters. |

All these files are presented on Figure 4.1-1.
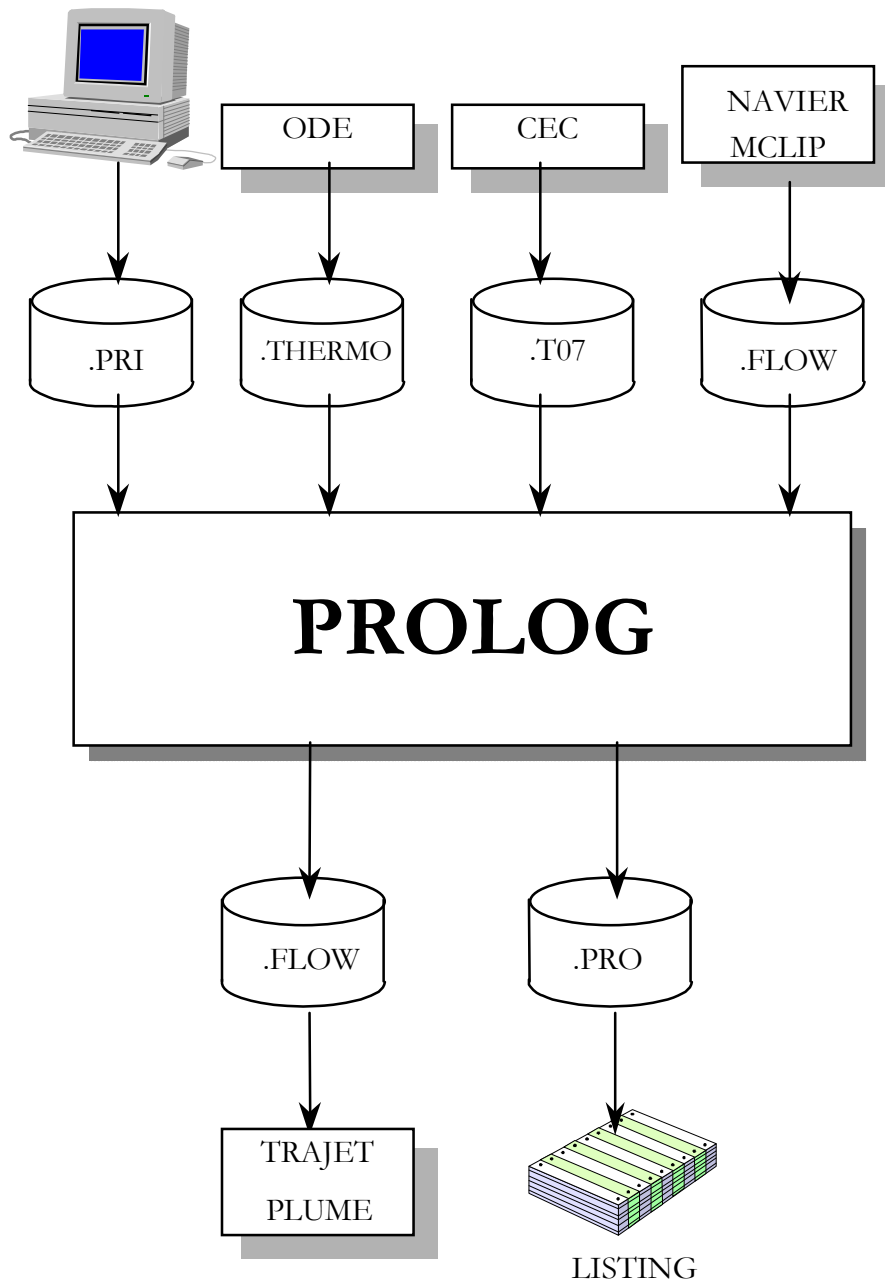
*Figure 4.1-2: PROLOG architecture.*

## 4.2 PROLOG INPUT FILES DESCRIPTION

### 4.2.1 .THERMO file

This file is the interface file to ODE. Gas table giving, versus the temperature: H, $W_{mol}$, $\gamma$, T, P, $C_p$, $\mu$, Pr.

### 4.2.2 .T07 file

This file contains the thermodynamic characteristics (mass, molar fraction, cross section, number of degrees of freedom) of each group of species. It can be created by the CEC module or by the ODE module (nevertheless, the normal way is to use the CEC module to control the content of the .T07 file).

### 4.2.3 .FLOW file

This file contains the characteristics (density, temperature, velocity) of the flow field inside and in the vicinity of the thruster. It is used to initiate the extension calculation at the limit of the computation domain. This file shall be created by the NAVIER or MCLIP module.

### 4.2.4 .PRI file

This is the user input file of PROLOG, composed of four namelists, giving the run parameters of the PROLOG module.

An example of the .PRI file is given on Figure 5.1-1 for the motor *"test"*.

The specification of the namelist in the "thruster name".PRI file must follow the order of the namelist description presented below.

**Format of the file :**

```
$GENERAL

[RUN_CONTINUE = continue]

[RUN_FREEMOL = freemol]

[RUN_BRIDGING = bridging]

$END

$CONTINUE

[N1C = n1c]                [N2C = n2c]                [NT = nt]

[SMAXC = smaxc]            [QNOZ = qnoz]              [QSL = qsl]

[DSMIN = dsmin]            [RLIP = rlip]              [BETA = beta]

[FRAC = frac]

[SMOOTHING_C = liss_c]     [WRITE_C = write_c]

[PSI = psi]

$END

$FREEMOL

[NSD = nsd]                [N1F = n1f]                [N2F = n2f]

[PSD1 = psd1]              [PSD2 = psd2]              [SMAXF = smaxf]

[IRAYMAX = iraymax]        [ISEED = iseed]            [BIRDLIM = birdlim]

[QZ=qz]                    [QR=qr]                    [FTYPE = ftype]

[RUN_CARTESIAN=run_cratesian]

[RUN_STREAMLINES=run_streamlines]

[SMOOTHING_F = smoothing_f]

[WRITE_FC = write_fc]      [WRITE_FS = write_fs]

[NISD = nisd]

$END

$BRIDGING

[BIRD1 = bird1]            [BIRD2 = bird2]

[SMOOTHING_B=smoothing _b]

[WRITE_B = write_b]

$END
```

### 4.2.4.1    Namelist $GENERAL

**Purpose:**

General definition of the run to be performed.

**Description :**

RUN_CONTINUE: Parameter to specify whether the user wants to perform a calculation with continuum regime assumption.

| | |
|---|---|
| Type: | logical |
| Range: | TRUE, FALSE |
| Default: | 1 |
| Unit: | None |
| Note: | TRUE if continuum calculation is requested |
| | FALSE if continuum calculation is not requested |

RUN_FREEMOL: Parameter to specify whether the user wants to perform a calculation with free molecular regime assumption.

| | |
|---|---|
| Type: | logical |
| Range: | TRUE, FALSE |
| Default: | 1 |
| Unit: | None |
| Note: | TRUE if free molecular calculation is requested |
| | FALSE if free molecular calculation is not requested |

RUN_BRIDGING: Parameter to specify whether the user wants to perform a calculation with transitional regime assumption.

| | |
|---|---|
| Type: | logical |
| Range: | TRUE, FALSE |
| Default: | 1 |
| Unit: | None |
| Note: | TRUE if bridging calculation is requested |
| | FALSE if bridging calculation is not requested |

### 4.2.4.2    Namelist $CONTINUE

**Purpose:**

Input data for PROLOG continuum flow field computation.

**Description:**

N1C:            Number of points on each gas streamline.

    Type:            integer

    Range:           2 < N1C < 500

    Default:         100

    Unit:            None

N2C:            Number of gas streamlines.

    Type:            integer

    Range:           2 < N2C < 100

    Default:         30

    Unit:             None

NT:             Number of points on each gas streamline for the expansion computation.

    Type:            integer

    Range:           2 < NT < 1000

    Default:         600

    Unit:            None

SMAXC:          Distance of the flow field extension in the curvilinear abscissa along the streamlines.

    Type:            real

    Range:           SMAXC > 0

    Default:         20

    Unit:            meter

QNOZ:                     Geometrical progression coefficient at the nozzle exit, defining the distribution of the streamlines at the nozzle exit.

    Type:                     real

    Range:                    0 < QNOZ < 1.

    Default:                  0.87

    Unit:                     None

    Note:                     The streamlines must be narrowed near the nozzle lip.


QSL:                      Geometrical progression coefficient along the streamlines, defining the distribution of the points along the streamlines.

    Type:                     real

    Range:                    QSL > 1

    Default:                  1.15

    Unit:                     None

    Note:                     The distribution of the points on the streamlines must be narrowed near the nozzle.


DSMIN:                    Distance between two points of a streamline in the initial domain interpolation, before the redistribution of the points along the streamlines.

    Type:                     real

    Range:                    dsmin > 0

    Default:                  0.005

    Unit:                     meter


BETA:                     Angle of the arc of the circle describing the nozzle lip.

    Type:                     real

    Range:                    beta > 0

    Default:                  200

    Unit:                     degree

FRAC:                    Fraction number between the number of streamlines from the nozzle exit and the total number of streamlines (N2C includes the streamlines from the nozzle lip).

        Type:                    real

        Range:                   $0 < frac < 1$

        Default:                 0.8

        Unit:                    None


SMOOTHING_C:        Continuum flow calculation smoothing parameter.

        Type:                    logical

        Range:                   TRUE, FALSE

        Default:                 1

        Unit:                    None

        Note:                    TRUE if smoothing is requested

                              FALSE if smoothing is not requested


WRITE_C:                Continuum mean flow calculation printing parameter.

        Type:                    logical

        Range:                   TRUE, FALSE

        Default:                 1

        Unit:                    None

        Note:                    TRUE if printing is requested

                              FALSE if printing is not requested


PSI:                    Gas stream function for each streamline

        Type:                    real

        Range:                   $0 < psi < 1$

        Default:                 linear distribution by PROLOG

        Unit:                    None

        Note:                    The number of values of the stream function must be the same as N2C, and are given separated by commas.

### 4.2.4.3    namelist $FREEMOL

**Purpose:**

Input data for PROLOG free molecular flow field computation.

**Description:**

N1F:                    Number of points on the Cartesian mesh on the Z-axis (thruster axis)

      Type:                    integer

      Range:                  1 < N1F < 500

      Default:                 100

      Unit:                    None

N2F:                    Number of points on the Cartesian mesh on the R-axis (thruster radius axis)

      Type:                    integer

      Range:                  1 < N2F < 100

      Default:                 50

      Unit:                    None

SMAXF:                  Distance of the flow field extension in the Cartesian mesh

      Type:                    real

      Range:                  smaxf > 0

      Default:                 20

      Unit:                    meter

      Note:                    SMAXF must be at least at the value of the continuum SMAXC extension distance to be able to interpolate the free molecular results into the continuum streamlines-based mesh.

IRAYMAX:        Number of rays emitted from each element of freezing surface

> Type:           integer
>
> Range:          iraymax > 0
>
> Default:        10000
>
> Unit:           None
>
> Note:           The highest IRAYMAX the better but the longer computation time

ISEED:          Initial random seed value used and propagated by the random number generator.

> Type:           integer
>
> Range:          iseed > 0
>
> Default:        4321
>
> Unit:           None
>
> Note:           A change of the initial value ISEED modifies the sequence of the random number.

QZ:             Geometrical progression coefficient at the Z-axis of the Cartesian mesh, defining the distribution of the points in the two directions of the axis from the origin Z=0.

> Type:           real
>
> Range:           $0 < qz < 1$
>
> Default:        0.99
>
> Unit:           None
>
> Note:           The distribution of points must be closely near the thruster. The cells should not be too stretched. The ideal shape of the mesh cells is square.

QR:                 Geometrical progression coefficient at the R-axis of the Cartesian mesh, defining the distribution of the points in the positive direction of the axis from the origin R=0.

|           |                                                                                                      |
|-----------|------------------------------------------------------------------------------------------------------|
| Type:     | real                                                                                                 |
| Range:    | 0 < qr < 1                                                                                           |
| Default:  | 0.99                                                                                                 |
| Unit:     | None                                                                                                 |
| Note:     | The distribution of points must be closely near the thruster. The cells should not be too stretched. The ideal shape of the mesh cells is square. |

RUN_CARTESIAN: Free molecular mean flow regime execution parameter in Cartesian based mesh.

|           |                                                      |
|-----------|------------------------------------------------------|
| Type:     | logical                                              |
| Range:    | TRUE, FALSE                                          |
| Default:  | 1                                                    |
| Unit:     | None                                                 |
| Note:     | TRUE if Cartesian based mesh execution is requested  |
|           | FALSE if Cartesian based mesh execution is not requested |

RUN_STREAMLINES:  Free molecular mean flow regime execution parameter in streamlines-based mesh.

|           |                                                           |
|-----------|-----------------------------------------------------------|
| Type:     | logical                                                   |
| Range:    | TRUE, FALSE                                               |
| Default:  | 1                                                         |
| Unit:     | None                                                      |
| Note:     | TRUE if streamlines-based mesh execution is requested     |
|           | FALSE if streamlines-based mesh execution is not requested |
|           | In any case, the free molecular calculation is always done in the Cartesian mesh and then the results are interpolated in the streamlines-based mesh if RUN_STREAMLINES is set to TRUE. |

SMOOTHING_F:    Free molecular flow calculation smoothing parameter.

    Type:          logical

    Range:          TRUE, FALSE

    Default:         1

    Unit:          None

    Note:          TRUE if smoothing is requested

                      FALSE if smoothing is not requested

WRITE_F:    Free molecular flow calculation printing parameter.

    Type:          logical

    Range:          TRUE, FALSE

    Default:         1

    Unit:          None

    Note:          TRUE if printing is requested

                      FALSE if printing is not requested

FTYPE:    Free molecular flow calculation control parameter, defining the previous calculation (before the use of PROLOG).

    Type:          integer

    Range:          0, 1, 2

    Default:

    Unit:          None

    Note:          0 unknown

                      1 if MCLIP is previously used

                      2 if NAVIER is previously used

BIRDLIM:      Bird number defining the freezing surface (from which the rays are emitted)

     Type:      integer

     Range:      0 < BIRDLIM < +inf

     Default:      0.1 ( pas sûr)

     Unit:      None

     Note:      the BIRDLIM should correspond to the border of the continuum field. The Ray Tracing method is then used in every point of the mesh where the Bird number B is such that: B>BIRDLIM. If MCLIP is used before PROLOG, then the BIRDLIM automatically corresponds to the limits of the MCLIP mesh.

#### 4.2.4.4 namelist $BRIDGING

**Purpose:**

Input data for PROLOG bridging flow field computation.

**Description:**

BIRD1:      Inferior Bird number limit corresponding to the continuum / transitional transition

     Type:      real

     Range:      BIRDLIM ≤ bird1 < +Inf

     Default:      0.1

     Unit:      None

BIRD2:      Superior Bird number limit corresponding to the transitional / free molecular transition

     Type:      real

     Range:      bird1 < bird2 < +Inf

     Default:      2.

     Unit:      None

SMOOTHING_B: Bridging flow calculation smoothing parameter.

      Type:              integer

      Range:            TRUE, FALSE

      Default:          1

      Unit:              None

      Note:             TRUE if smoothing is requested

                            FALSE if smoothing is not requested

WRITE_F: Bridging flow calculation printing parameter.

      Type:               integer

      Range:            TRUE, FALSE

      Default:          1

      Unit:              None

      Note:             TRUE if printing is requested

                            FALSE if printing is not requested

## 4.3 PROLOG OUTPUT FILES DESCRIPTION

### 4.3.1 .PRO file

This is a listing file containing a summery of the input parameters and some information concerning the progress of the run.

The output listing file is composed of four parts.

- The description of the run parameters from the user .PRI file.

- A summary of the .T07 file.

- A summary of the .FLOW file.

- A summary of the output .FLOW files depending on the run parameters:

  ➢ A summary of the continuum flow of the C.FLOW file:

   ✓ The main characteristics of the mesh.

   ✓ The total mass flow rate conservation and the mass flow rate conservation along the streamlines

  ➢ A summary of the free molecular flow in the Cartesian mesh of the FC.FLOW file:

   ✓ The main characteristics of the mesh.

  ➢ A summary of the free molecular flow in the streamline mesh of the FS.FLOW file:

✔ The main characteristics of the mesh.

➢ A summary of the bridging flow of the B.FLOW file:

✔ The main characteristics of the mesh.

An example of .PRO file is given at Figure 5.1-1.

```
    -----------------------------------------
    SPECIES PROPERTIES DESCRIPTION  .T07 FILE
    -----------------------------------------

    Reference temperature : 1141.6600342

    Number of groups :   1

    Group name    Molecular fraction    Molecular mass     Diameter      Degrees of freedom
      MOY          .1000000E+01          .1774527E-25      .2042760E-09        2.6238000


    --------------------------------------
    RUN PARAMETERS DESCRIPTION  .PRI FILE
    --------------------------------------

    $NAMELIST GENERAL
    -----------------
        CONTINUUM FLOW FIELD EXECUTION PARAMETER              RUN_CONTINUE = T
        FREE MOLECULAR FLOW FIELD EXECUTION PARAMETER         RUN_FREEMOL  = T
        BRIDGING FLOW FIELD EXECUTION PARAMETER               RUN_BRIDGING = T

    $NAMELIST CONTINUE
    -----------------
        CONTINUE FLOW FIELD PRINT PARAMETER                   WB     = T
        NUMBER OF POINTS BY STREAMLINE                        N1C    =    100
        NUMBER OF STREAMLINES                                 N2C    =     30
        NUMBER OF                                             NT     =    300
        CONTINUUM FLOW FIELD EXTENSION LENGHT                 SMAXC  = 0.5000000E+01
        GEOMETRIC PROGRESS COEFFICIENT AT THE NOZZLE EXIT     QNOZ   = 0.8700000E+00
        GEOMETRIC PROGRESS COEFFICIENT ALONG THE STREAMLINES  QSL    = 0.1150000E+01
        DISTANCE BETWEEN 2 POINTS OF A STREAMLINE             DSMIN  = 0.3000000E-03
        NOZZLE LIP                                            RLIP   = 0.3000000E-03
        NOZZLE LIP ANGLE                                      BETA   = 0.1900000E+03
        FRACTION NUMBER OF POINTS NOZZLE EXIT/NOZZLE LIP      FRAC   = 0.7500000E+00
    -----------------
        FREE MOLECULAR FLOW FIELD EXECUTION PARAMETER
        CARTESIAN MESHGRID                                    RUN_FC = T
        FREE MOLECULAR FLOW FIELD EXECUTION PARAMETER
        STREAMLINES MESHGRID                                  RUN_FS = T
        FREE MOLECULAR FLOW FIELD PRINTING PARAMETER
        CARTESIAN MESHGRID                                    WFC    = F
        FREE MOLECULAR FLOW FIELD PRINTING PARAMETER
        STREAMLINES MESHGRID                                  WFS    = T
        NUMBER OF RAYS SHOT FROM EACH PEACE OF SURFACE        IRAYMAX =  10000
        RANDOM SEED                                           ISEED  =   4321
        BIRD NUMBER LIMIT                                     BIRDLIM = 0.1000000E+00
        FREE MOLECULAR FLOW FIELD EXTENSION LENGHT            SMAXF  = 0.5000000E+01
        GEOMETRIC PROGRESS COEFFICIENT ALONG THE Z-AXIS       QZ     = 0.9700000E+00
        GEOMETRIC PROGRESS COEFFICIENT ALONG THE R-AXIS       QR     = 0.9700000E+00

    $NAMELIST BRIDGING
    ------------------
        BRIDGING FLOW FIELD PRINT PARAMETER                   WB     = T
        LOWER BRIDGING BIRD NUMBER LIMIT                      BRD1   = 0.5000000E+00
        UPPER BRIDGING BIRD NUMBER LIMIT                      BRD2   = 0.2000000E+01
```

```
                    *******************************************
                        PROLOG COMPUTATION OF THE THRUSTER
                    *******************************************


       ------------------------------------------
       INPUT FLOW-FIELD DESCRIPTION  .FLOW FILE
       ------------------------------------------

       NOZZLE DESCRIPTION
       ------------------
           THROAT RADIUS       = 0.7937500E-03 M
           THRUST              = 0.2038445E+01 N
           MASS FLOW RATE      = 0.8807816E-03 KG/S
           EXIT RADIUS         = 0.7099100E+01 R*
           THROAT/EXIT LENGTH  = 0.1526400E+02 R*
           IDEAL GAS                                       NGAS =    3


       FLOW-FIELD PARAMETERS
       ---------------------
           NUMBER OF POINTS BY STREAMLINE               NPT = 145
           NUMBER OF STREAMLINES                        NSL =  49
           NUMBER OF VARIABLES OF THE FLOW-FIELD FILE   NVT =  12
```

***Figure 4.3-1 : Example of PROLOG output file***

### 4.3.2    .FLOW files

These files contain the characteristics (density, temperature, velocity) of the flow field computed by the PROLOG module. It allows the visualisation of the flow field using the TRAJET module. Each file corresponds to one type of flow regime:

- C.FLOW: continuum regime flow.

- FC.FLOW: free molecular regime flow in a Cartesian mesh.

- FS.FLOW: free molecular regime flow in the streamlines-based mesh.

- B.FLOW: bridging flow.

## 5    HOW TO USE PROLOG

The aim of this chapter is to present the use of the PROLOG module on a real case and to give some advises to the user.

### 5.1    APPLICATION CASE

A complete case of a PROLOG execution is presented in this paragraph. The application case is provided for the test thruster.

#### 5.1.1    External input files

To perform the computation of the application case, the user shall have in the current directory:

- A test.FLOW file computed by the MCLIP module.

- A test.THERMO file computed by the ODE or CEC module.

- A test.T07 file computed by the CEC module. An example of the .T07 file is given in the CEC application manual.

#### 5.1.2    User input file

The user input file .PRI, test.PRI, provides the run parameters for the PROLOG computation. To generate this file, the user can edit the .PRI file using the PLUMFLOW interface or any other text editor. To edit the file with the PLUMFLOW interface, after selecting the thruster test, click on **Edit input file**, then on **PROLOG**. The user can then write the following instructions:

```
$GENERAL
 RUN_CONTINUE=.TRUE.,RUN_FREEMOL=.TRUE.,RUN_BRIDGING=.TRUE.
$END
$CONTINUE
 N1C=100, N2C=30, NT=300, SMAXC=5., QNOZ=0.87 ,QSL=1.15
 DSMIN=3.E-4, RLIP=3.E-4, BETA=190., FRAC=0.75,
 PSI = .00 , .10 , .20 ,.30 ,.40 ,.50 ,.60 ,.65 ,.69 ,.71 ,
     .725 , .733 , .75 ,.76  ,.77 ,.77 ,.775 ,.777 ,.793 ,.795117,
     .7955 ,.7957 ,.7959 ,.796 ,.797 ,.798 ,.80 ,.83, .85 ,.93,.95,.98,.99
$END
$FREEMOL
 N1F=100
 N2F=50
 SMAXF=5.,IRAYMAX=10000, ISEED=4321
 BIRDLIM = 0.1, QZ=0.97, QR=0.97
 WRITE_FC = .FALSE.
$END
$BRIDGING
 BIRD1=0.5, BIRD2=2.
$END
```

***Figure 5.1-1 : Example of input file for the test thruster***

To save the file, click on the **save** button, then click on the **quit** button to quit.

### 5.1.3   PROLOG execution

To perform the PROLOG computation, click on the **PROLOG** ON/OFF button in the main menu.

After the run of the PROLOG module, the user can edit the .PRO output listing file, using the PLUMFLOW integrated editor. To edit the test.PRO file, click on **Edit output file** on the main menu, then on **PROLOG**. A description of the .PRO file is provided in paragraph 4.3.1.

In order to check the validity of each step of the computation, it would be helpful to perform the computation in three steps, corresponding to the three flow regimes. After each execution, the user can edit the output listing test.PRO file.

### 5.1.3.1  Flow field visualisation

A visualisation of the flow field computed by PROLOG can be performed using the TRAJET module of PLUMFLOW. To do so in the PLUMFLOW interface, choose the thruster name, and then click on *isovalue contours.* The user can see the different flow field parameters.

### 5.1.3.2  Continuum regime calculation

To perform a visualisation of the flow field parameters follow the instructions in §5.1.3.1 with the thruster name testC. The results are presented at Figure 5.1-2.
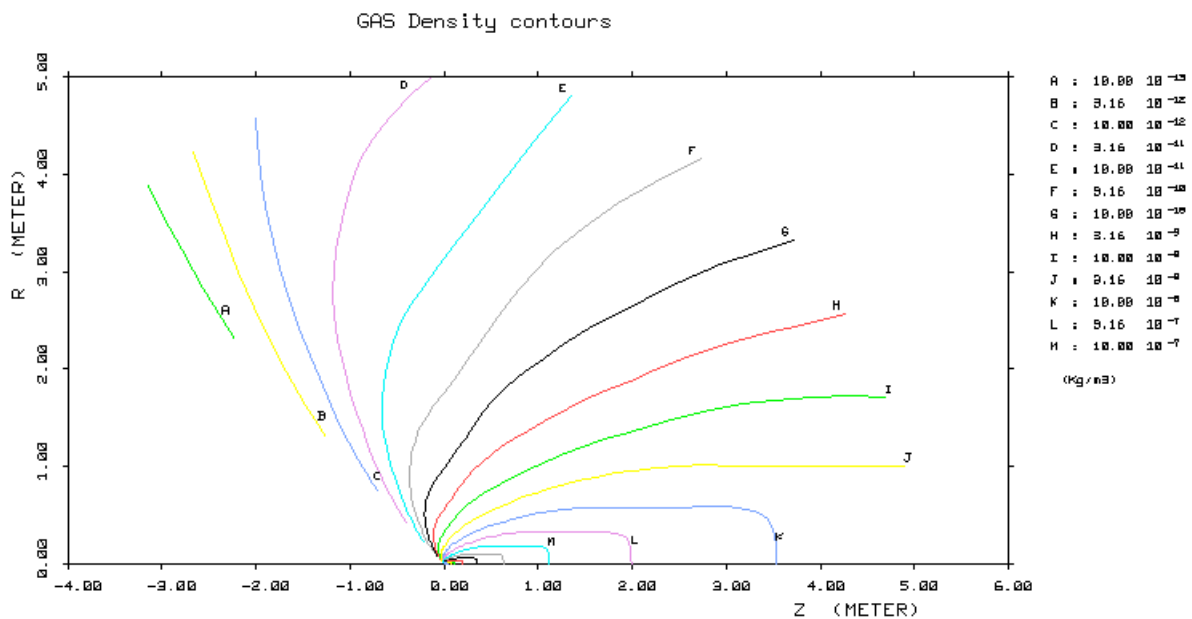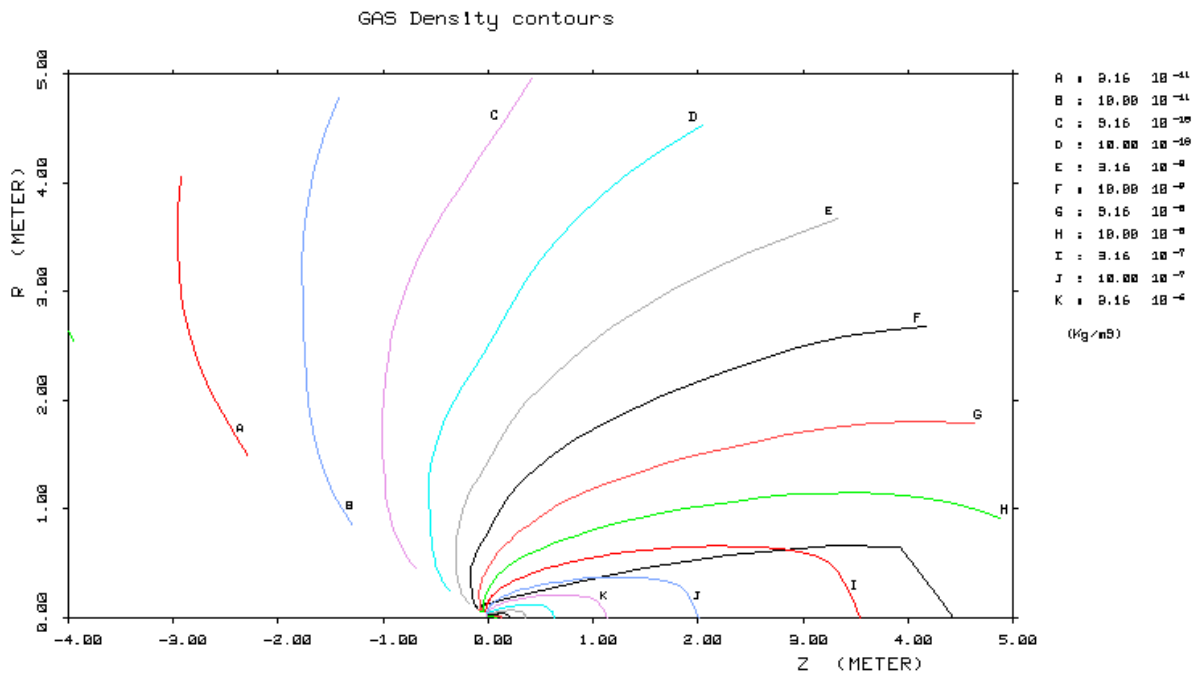


*Figure 5.1-2 : Flow field density after continuum regime calculation*

### 5.1.3.3  Free molecular regime calculation

The second step of calculation is the computation of the free molecular flow field regime. This execution if performed is the RUN_FREEMOL parameter is equal to TRUE. The user can choose the Cartesian sub-domain to be visualised by the TRAJET module, by setting the NISD parameter to the number of the sub-domain required. For example, we choose the third sub-domain, NISD=3.

The user can then visualise the flow field parameters following the instructions given in §5.1.3.1, with the thruster name testFS for the results along streamlines. The iso-density results are presented at Figure 5.1-3.
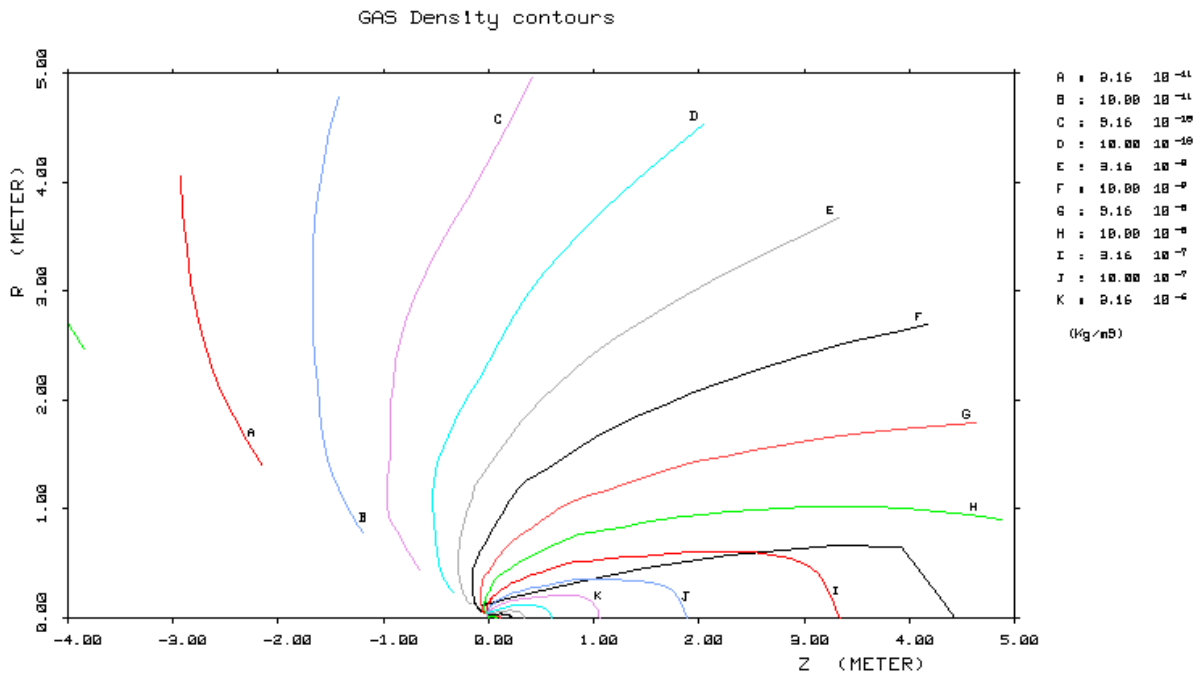
*Figure 5.1-3 : Flow field density after free molecular regime calculation*

<u>Remark</u>: The results computed on the Cartesian mesh can be also visualised from the testFC file. This visualisation is less exploitable because limited to the NISD block.

### 5.1.3.4 Bridging between continuum and free molecular

The third step of calculation is to compute the bridging between continuum and free molecular regimes. This execution if performed is the RUN_FREEMOL parameter is equal to TRUE.

To perform a visualisation of the flow field parameters follow the instructions in §5.1.3.1 with the thruster name testB. The iso-density results are presented at Figure 5.1-4.

***Figure 5.1-4 : Flow field density after bridging calculation***

## 5.2   ADVISES TO THE USER

### 5.2.1   On the continuum flow regime computation

The radius RLIP and the angle BETA of the arc of the thruster lip are important parameters for the continuum flow regime computation, because it influences the velocity directions, especially for the backflow, thus the streamlines distribution. RLIP must be at minimum value as possible, and BETA must be at maximum value as possible to allow maximum backflow area.

The table **mass flow rate conservation** shows the importance of the flow rate loss, integrated at a given point of the streamlines meshing, due to the accumulated inaccuracies of the linear interpolations along the streamlines calculation and the remeshing of the points.

The source-flow method insures the rigorous mass flow rate conservation, so that the mass flow rate does not change along the streamlines in the extension area.

### 5.2.2   On the free molecular regime flow computation

There are different ways to increase the precision of the free molecular flow regime computation, by increasing:

- The number of cells of the Cartesian mesh,

- The number of emitted rays,

- The number of subdomains for better precision nears the thruster nozzle.

It is important to choose a sufficiently thin mesh to perform a calculation, but it is also important to have high value of the number of emitted rays.

In the Cartesian mesh, the cells should be as squared as possible in order to have a good interpolation of the results in the streamlines based mesh. The user is recommended to set QR and QZ carefully.

To save time, the IRAYMAX parameter can be set to 1 when creating the mesh.

The most difficult area to obtain a nice precision is near the thruster nozzle, so it is generally useful to set the number of sub-domains at least at 2, even preferably at 3.

### 5.2.3    On the bridging computation

Be careful about the continuity of the flow-field parameters in the transition between the continuum flow regime and the transitional flow regime, and between the transitional flow regime and the free molecular flow regime, especially near the thruster nozzle.

An easy way of checking whether the bridging is successfully achieved is to visualize the iso-BIRD corresponding to bird1 and bird2 and see if the results-for instance the density-are bridged between the two iso-contours. The density is normally the same as the one from continuum flow regime in the areas where the bird number is lower than bird1, and anywhere else where the bird is greater than bird2 the results should be the same as those in free molecular flow regime.

# 6    THEORETICAL ANALYSIS

The aim of this chapter is to provide some theoretical analysis of the PROLOG module. For each flow regime, important theoretical aspects and methods used are presented.

## 6.1    ASSUMPTIONS

## 6.2    NOMENCLATURE

$\beta$        statistical temperature

$\gamma$        perfect gas coefficient (adim)

$\lambda$        mean free path (m)

$\mu$        viscosity at reference temperature

$\rho$        density (kg/m³)

$\rho_i$        isentropic stop density (kg/m³)

$\theta$        random angle of the tangential velocity direction (radian)

$A$        freezing surface (m²)

$Bird$        Bird number (adim)

$CAPN$   viscosity variation superscript (adim)

$d$        mass flow rate (kg/s)

$d_{ray}$        mass flow rate carried by the emitted ray (kg/s)

$f_x$        cumulative distribution function of the variable x (adim)

$F_x$        cumulative distribution function of the variable x (adim)

$k$        Boltzmann constant

$M$        Mach number (adim)

$m$        mean molecular mass (kg)

$P_s$        static pressure (Pa)

$P_d$        Dynamic pressure (Pa)

$r$        Perfect gas constant

$s$        Curvilinear abscissa along the streamlines (m)

$S$        Molecular speed ratio (adim)

$T_m$        Mean temperature (K)

$T_r$        Viscosity reference temperature (K)

$T_i$        Isentropic stop temperature (K)

$T_1, T_2, T_3$      Kinetic temperature in the three cartesian axis (K)

$T$      Temperature or mean kinetic temperature (K)

$t_{res}$      Residence time of a ray crossing a cell of the mesh

$V$      Mean velocity (m/s)

$V_{mesh}$      Volume of the cell of the mesh (m³)

$V_i$      Velocity in the i-axis direction (m/s)

$\overline{V}$      Mean velocity module (m/s)

$\overline{V_i^2}$      Mean square velocity in the i-axis direction (m/s)

$V_n$      Normal velocity module from the freezing surface (m/s)

$V_t$      Tangential velocity module from the freezing surface (m/s)

$V_{t1}$      tangential velocity in the 1-axis from the freezing surface (m/s)

$V_{t2}$      tangential velocity in the 2-axis from the freezing surface (m/s)

## 6.3   CONTINUUM FLOW REGIME

The continuum flow regime needs two steps calculating the flow parameters:

- Mesh generation,
- Flow field extension assuming isentropic expansion.

To improve the regularity of the streamlines mesh, the points are then re-distributed on each streamline according to a geometrical progression law. The flow parameters are computed at new point by interpolation between two old points.

### 6.3.1   Mesh generation

The flow field of the continuum regime is determined on a streamlines-based mesh computed from the initial NAVIER or MCLIP computation domain, and extended using a source-flow method.

- Streamlines determination in the initial domain: is performed by a bi-linear interpolation between 4 points of a cell, from the NAVIER or MCLIP computation domain. They are built point after point, following the velocity direction, and being considered as iso-mass-flow-rate lines.

- Source-flow method in the frontflow expansion: the streamlines, computed in the initial domain, are extended in the far flow-field by the source-flow method up to the SMAX distance, defined by the user. They are extended, by straight lines passing through the source-points. The source-point is considered in the centre of the nozzle exit plan (on the axis), which allows knowing the flow up to an angle of $\pi/2$ between the velocity direction and the thruster axis.

- Backflow expansion: the streamlines are extended by straight lines with the direction of the last point of the streamline interpolated in the initial domain.

### 6.3.2    Isentropic expansion along the streamlines

The flow parameters are computed in the extended domain assuming isentropic expansion of the gas.

$$\frac{T_i}{T} = 1 + \frac{\gamma - 1}{2} M^2 \quad (6.3.2\text{-}1)$$

$$\frac{\varrho_i}{\varrho} = \left( 1 + \frac{\gamma - 1}{2} M^2 \right)^{\frac{1}{\gamma - 1}} \quad (6.3.2\text{-}2)$$

$$\frac{dM}{M} = \frac{1 + \frac{\gamma - 1}{2} M^2}{1 - M^2} \frac{dA}{A} \quad (6.3.2\text{-}3)$$

$$V = \frac{M}{\sqrt{\gamma r T}} \quad (6.3.2\text{-}4)$$

$$Ps = \varrho r T \quad (6.3.2\text{-}5)$$

$$Ps = \frac{1}{2} \varrho V^2 \quad (6.3.2\text{-}6)$$

$$\lambda = \frac{\mu.\left(T_m.T_r\right)^{CAPN}}{\varrho} \sqrt{\frac{\pi M}{2kT_m}} \quad (6.3.2\text{-}7)$$

$$B_{ird} = \frac{\lambda}{\varrho} \left| \frac{\partial \varrho}{\partial s} \right| \quad (6.3.2\text{-}8)$$

### 6.3.3    Multi-species computation

In continuum flow regime, the multi-species computation is determined with the continuum mean flow regime by giving the density a weight corresponding to the molecular fraction of each species of the gas. The other flow parameters (temperature, velocity) do not have multi-species value and are given the mean flow parameters value.

### 6.4    FREE MOLECULAR FLOW REGIME

As described before (see §3.2), the free molecular flow regime uses a ray-tracing method. This paragraph presents the theoretical aspects of the molecules introduction from the freezing surface, and the calculation of the macroscopic flow parameters in each cell of the mesh. The Figure 6.4-1 presents the free molecular computation principle.
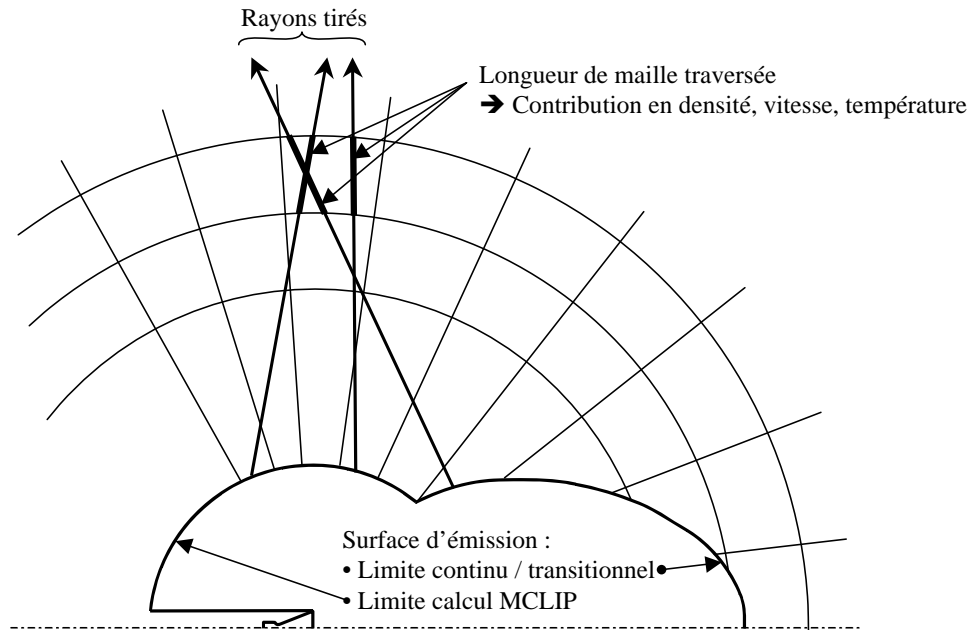
**Figure 6.4-1 : Free molecular computation method**

The different steps of the computation described below are:

- Freezing surface determination,
- Molecules introduction from the freezing surface,
- Flow parameters computation in each cell of the mesh.

### 6.4.1 Mesh generation

The Cartesian mesh is divided into subdomains.

### 6.4.2 Freezing surface

The freezing surface is the limit between the continuum flow regime and the free molecular flow regime. It is determined by the points of the streamlines of the continuum extension flow field where the Bird parameter is calculated as having the Bird parameter value defined by the user. The freezing surface is calculated to be convex to avoid the emitted rays of particles to interact with the freezing surface.

In the case of a MCLIP input .FLOW file, the freezing surface is calculated taking into account the MCLIP computation domain which is assumed not to have to be recomputed by the free molecular regime calculation.

### 6.4.3 Molecules introduction

Each emitted ray from the freezing surface carries a representative sample of molecules. This paragraph presents the characteristics to be calculated for each ray: emission coordinates, statistical temperature,

emission velocity and exit mass flow rate. The methods used are based on the generation of random numbers and the use of the velocity distribution function.

### 6.4.3.1   Velocity distribution function

The gas properties in equilibrium can be described by the Maxwellian distribution function:

$$f = \frac{\beta^3}{\pi^{\frac{3}{2}}} \exp\left(-\beta^2 V^2\right) \text{ (6.4.3-1)}$$

where: $\beta = \sqrt{\dfrac{m}{2kT}}$ is the statistical temperature, $V$ the velocity, $T$ the thermodynamic temperature, $m$ the molecular mass and $k$ the Boltzmann constant.

### 6.4.3.2   Random emission point coordinates

The emission point coordinates are assumed to be distributed uniformly along the freezing surface. The sampling uses random numbers and the method need different equations according to the surface type, cylinder, disc or cone. The surfaces are axially symmetric surface, one need then just two points coordinates in a plan including the symmetry axis. This paragraph presents the general method for sampling the shooting point. The method is then applied for the three different surface types used in the PROLOG module.

Let $P_1(Z_1,R_1)$ and $P_2(Z_2,R_2)$ be the two points describing the surface, and $P(Z,R)$ the emission point. The probability of locating a point at a point P is proportional to the element of surface $dS$ around this point $P$:

$$P = \frac{dS}{S_{total}} \text{  (6.4.3-2)}$$

The different steps of the computation are:

- Generation of a random number *rand* between *0* and *1*

- Calculation of the abscissa $Z$ with the equation :

$$rand = P(Z) = \int_{Z1}^{Z} p(x)dx \text{  (6.4.3-3)}$$

- Calculation of the fraction giving the abscissa relation :

$$a = \frac{Z - Z1}{Z2 - Z1} \text{  (6.4.3-4)}$$

- Calculation of the ordinate $R$ with the same relation as the one for the abscissa :

$$R = a.R1 + (1 - a).R2 \text{  (6.4.3-5)}$$

### 6.4.3.3    Introduction velocity

The calculation of the random velocity value at the freezing surface uses the velocity distribution function. The three entering (in the free molecular region) velocity directions, one in the external normal to the freezing surface direction, and two in the tangential to the freezing surface direction, are determined as following:

- Normal velocity: the normal velocity value is calculated using the acceptance-rejection method:

The uniformly distributed value of $V_n$ is given by:

$$V_n = a + rand.(b - a) \quad (6.4.3-6)$$

where *rand* is a random number, with a and b set as arbitrary finite cut-off values in place of the real limits of $-\infty$ to $+\infty$. The distribution function is then calculated for the value of $V_n$ determined before:

$$f_{\beta^2 V_n^2} = \exp\left(-\beta^2 V_n^2\right) \quad (6.4.3-7)$$

The next random number *rand* is then generated and if $f_{\beta^2 V_n^2} > rand$, $V_n$ is accepted. If $f_{\beta^2 V_n^2} < rand$ the value of $V_n$ is rejected and the process is repeated until a value is accepted.

- Tangential velocities: the two tangential velocity values are given using a direct method of sampling from the normal distribution:

Using polar coordinates, one can rewrite the distribution function as:

$$f_{\beta^2 V^2} = \exp\left(-\beta^2 V^2\right) \quad (6.4.3-8)$$

where $\beta^2 V^2$ is distributed between *0* and $\infty$, and the cumulative distribution function is

$$F_{\beta^2 V^2} = 1 \quad \exp\left(-\beta^2 V^2\right) \quad (6.4.3-9)$$

A pair of value of *r* and $\pi$ may then be calculated using random number *rand*. The $\theta$ angle is uniformly distributed between *0* and *2π*:

$$\theta = 2.\pi.rand \quad (6.4.3-10)$$

The tangential velocity module $V_t$ is given by equation (6.4.2.3-2), setting $F_{\beta^2 V^2}$ to *rand* random number:

$$Vt = \frac{\sqrt{(-\ln(rand))}}{\beta} \quad (6.4.3-11)$$

Finally, the two tangential velocity components are:

$$V_{t1} = V_t \cos\theta \quad (6.4.3-12)$$

$$V_{t2} = V_t \sin\theta \quad (6.4.3-13)$$

#### 6.4.3.4 Exit mass flow rate

The exit mass flow rate corresponds to the mass flow rate outgoing the freezing surface, in the free molecular region. The exit number flux is given by:

$$\dot{N} = n \int_{\infty}^{+\infty} \int_{\infty}^{+\infty} \int_{\infty}^{+\infty} u.f\,.du.dv.dw \quad (6.4.3\text{-}14)$$

Where $n$ is the number density, $f$ the Maxwellian distribution function, and $u$, $v$, $w$ are the velocity in the three Cartesian axis. Then, replacing the distribution function by its value and using the relation giving the density: $n = \dfrac{\varrho N}{m}$ where m is the molecular mass, the exit mass flow rate carried by each ray is given by:

$$d = \frac{\varrho A}{2\sqrt{\pi}\beta}\left[e^{S^2\cos^2\theta} + \sqrt{\pi}S\cos\theta\left(1 + erf(S\cos\theta)\right)\right] \quad (6.4.3\text{-}15)$$

where $S = V\beta$ is the molecular speed ratio.

Each ray carries a fraction of the mass flow rate given before. If a number of $N$ rays is emitted from an element of freezing surface, the mass flow rate of each ray from that surface element is:

$$d_{beam} = \frac{d}{N} \quad (6.4.3\text{-}16)$$

#### 6.4.4 Macroscopic flow field parameters

The emitted rays from the freezing surface are propagated throughout the whole mesh where each crossed cell is determined. The contribution of the rays in the flow parameters (density, velocity module, square velocity module and temperature in the three Cartesian axis) in each cell of the mesh is proportional to the length of the crossed cell. The macroscopic parameters of the flow field are determined by calculating the mean value of the parameters in each cell of the mesh:

$$\varrho = \frac{1}{V_{mesh}}\sum_{mesh} t_{res}.d_{beam} \quad (6.4.4\text{-}1)$$

$$V_i = \frac{\sum_{mesh} t_{res}.d_{beam}.V}{\sum_{mesh} t_{res}.d_{beam}} \quad (6.4.4\text{-}2)$$

$$\overline{V_i^2} = \frac{\sum_{mesh} t_{res}.d_{beam}.V^2}{\sum_{mesh} t_{res}.d_{beam}} \quad (6.4.4\text{-}3)$$

$$T_i = \frac{\left(\overline{V_i^2} - \overline{V_i}^2\right)}{k} \quad (6.4.4\text{-}4)$$

$$T = \frac{(T_1 + T_2 + T_3)}{3} \quad (6.4.4\text{-}5)$$

### 6.4.5   Multi-species computation

The multi-species computation in free molecular flow regime is determined with the same method as with the mean flow computation, and uses the freezing surface computed in the mean flow regime. The introduction characteristics carried by the rays are calculated with the results of the multi-species continuum flow regime.

## 6.5   BRIDGING

The bridging computation provides the flow field results in the whole extended domain taking into account the different flow regimes. The three calculated domains are given below:

- Transition regime flow field computation:  The transition regime flow field is determined by two Bird parameter values defined by the user, and the flow field parameters are calculated with a linear Bird-depending interpolation between the continuum regime flow field and the free molecular regime flow field.

- Continuum flow field domain: The continuum flow field domain is the one defined for the Bird parameter value less than the lower limit of the Bird parameter in the transition area, with the values of the flow field parameters in that domain computed before.

- Free molecular flow field domain: The free molecular flow field domain is the one defined for the Bird parameter value greater than the upper limit of the Bird parameter in the transition area, with the values of the flow field parameters in that domain computed before.

The bridging is computed interpolating the two flow regimes – continuum and free molecular regimes – previously computed, with the use of a function, as following:

$$F = F_{cont} + f(B_d).(F_{free} - F_{cont}) \quad (6.4.5\text{-}1)$$

Where $F$ can either be the density or the temperature or the velocity, and $f(B_d)$ is a function of the Bird number $B_d$, which value is fixed at 0 in the continuum domain, and 1 in the free molecular domain.

The $f(B_d)$ function used in the PROLOG module is a simple linear function of the Bird number.

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