

SYSTEMA ATOMOX

Version 4.9.3

User Manual

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1 Introduction

1.1 Foreword

The ATOMOX User's Manual describes how to perform an atomic oxygen analysis.

It contains all the key-information to understand and use the software. It is also intended as a reference manual.

1.2 Software Presentation

A good knowledge of temperature, total density, concentrations of gas constituents, and pressure, can be important for many space missions in the low-earth orbit regime, below 1000 km altitude.

ATOMOX software is an enhanced 3D numerical analysis tool for evaluation of atomic oxygen (and other species of the atmosphere) flux, fluence and material erosion, based on existing atmosphere and wind models. It involves mission and pointing modules, the ray-tracing technique and 2D and 3D visualization facilities.

All spacecraft surfaces are meshed into elements and the analysis is performed for each element. The mission and pointing modules provide the discretized location of the spacecraft together with its velocity with respect to the Earth. At the end of each orbital arc, orbital averaged or accumulated values are calculated which can be extrapolated when several arcs are specified.

The ray-tracing technique (Monte-Carlo technique) is used. It considers emitted rays from the surface of the satellite and detects if a given element is struck by the ray. Then, the ray can be followed by multiple reflections on the satellite surfaces (specular and diffuse reflectance taken into account). Outputs are:

- the total impacting flux and fluence,
- the absorbed flux and fluence,
- the direct impacting flux and fluence,
- the spacecraft material erosion,
- the mean impact velocity (amplitude and direction),
- the mean particle energy.

The model includes the effects of thermal motion of ambient particles in addition to the ambient atmospheric density and the velocity of the spacecraft. Thermal molecular motion can be responsible of erosion of surfaces that are shadowed during the mission.





2 Using the software

In this section, a simple case is detailed as a getting started, from generating a simple shape with Atomox properties to setup, up to the content of the resulting files.

2.1 Modeler

2.1.1 Material

There are no material library available with ATOX properties for now. The user can create one with its own properties, or directly go to the model properties to setup the value.

2.1.2 Model

In the model tab, the user can create a model, ranging from complex satellite assembly to a simple quadrangle. For all the possibilities regarding the model creation, please refer to the Systema User Manual. Here a simple rectangle is created, with the following definition.



Figure 1 – Model - Simple case – Geometry

Then the user can customize the ATOX properties of the shape in the Atomox tab.





General Atomox	
Coating	
Inherited configuration	(\$
Side management	Activity Overload Revert
Alike sides 🔶	Both sides 🔷 🖨
Alike sides	
Ray Emission	
- Emission	Overload Revert
Normal	
Inermo-optical	<select material=""> -</select>
— Absorptivity (alpha) —	Remove Revert
1	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
- Specularity	Remove Revert
0	
- Accommodation	Remove Revert
	₩
0	
Reaction Rate	Overload Revert
1e-24	

Figure 2 - Model - Simple case - Atomox properties

The properties that can be selected are:

- The inheritance of parent properties or local setup properties: if inherited is selected, the properties form the first parent will be applied. One or several of the ATOX properties can be modified locally, based on inherited properties. This is detailed below.
- Side Management: Work with the shape being considered as a whole (front and back), or as two separated entities, with each its properties.
- Activity allows: computation on both sides, positive only, negative only or no activity on the shape.
- Ray emission: Enforce a level of criticality for the number of ray computed on a shape. The number of corresponding rays can be setup in the processing tab (described later in the document).

Once these computation parameters are setup, physical properties can be enforced: the absorptivity, the specularity, the diffuse reflection, the accommodation and the reaction rate.

The sum of the absorptivity, the specularity and the diffuse reflection is equal to 1. The first two can be setup in the menu, and the diffuse reflection is computed from the absorptivity and the specularity.

The accommodation parameter is a coefficient that mitigates the diffuse reflection. It is here to model the transformation of energy at reemission of a particle, and take into account that kinetic energy is transformed in thermal energy. It is defined between 0 and 1. If accommodation is equal to 0, the transfer of energy from kinetic to thermal is not taken into account. If accommodation is equal to 1, all the kinetic energy of the

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particle is transformed, and the atom is not reemitted.

Finally the Reaction Rate is a material property that allow the computation of erosion rate at the end of the computation.

2.1.3 Meshing

Once the model is created and the Atomox parameters are setup, the meshing can be generated. The geometric meshing definition can be chosen from the definition of length/angle to a,b,c. For more information on the meshing definition, please refer to the definition in the Systema User Manual.

General		General	
MESHING PARAMETERS	Remove Revert	- MESHING PARAMETERS	Remove Revert
Method		Method	
Length	\$	Split a*b*c	•
Length	₩	a	₩
1	m	1	
Maximum Angle	₩	D 1	₩
30	dea		
	*	-	
Do not mesh			×
		Do not mesh	
LABEL	Overload Revert	LARTI	Overland Devert
Label		LABEL	Overload Revert
		Label	₩-

Figure 3 - Meshing - Simple Case

Atomox also has groups in order to get information about the result of the group only. The groups are defined on complete shapes, the user cannot create a group of only certain mesh of one shape. No parameters are needed in the groups, to know how to create this specific item please refer to the Systema User Manual.

General	
- REFERENCED OBJECT	Revert
Meshing group	
	Display browser
1 selected item	Add selection Remove selection
COMMENT	Add

2.2 Trajectory

Once every parameter has been set in the Modeler tab, the next step to define is the trajectory. Please refer to the Systema User Manual for the definition. An example of a parameter set is proposed in the figure below, in a General Keplerian orbit definition.

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ORBIT		Re	vert
General keplerian parameters			
Orbit reference			
Earth			\$
Ellipse definition	Semi major axis	K Excentricity	-
Semi major axis & excentricity 🗦	6800	km 0	
Ascending node definition	Ascer	nding node longitude	-
East longitude in inertial Gamma5	0 frame 😫 🛛 0		0
Inclination	₩ Argument of	the periapsis	-
99.4789	° 0		
Anomaly type	Anomaly		-
True anomaly	• 0		
Reference date			
Calendar date			\$
			<u> </u>
03/08/2021 00:00:00.000			~
START		Re	vert
Calendar date			
03/08/2021 00:00:00.000			
END		Re	evert
Revolution			
1			
INFORMATION			
Info: "New General keplerian" lasts	from 03/08/2021 (00:00:00.000 to 03/0	8/20

Figure 4 - Trajectory - Simple Case - Orbit definition

2.3 **Kinematics**

The following stage of setting up the simulation is to define the attitude of the satellite. Please refer to the Systema User Manual for a more detailed explanation. An example of a parameter set is proposed in the figure below. It is worth noticing that the velocity vector is a key parameter for Atomox computation, as the initial trajectory of Atomic Oxygen is coming in the velocity direction.





simple_case.syskin edition				ØX
Kinematics				
PHASES				
Default phase (default)			🔷 🗧 Edit	
General				
KINEMATIC LAW - Default phase				
Multiple laws				
Orbit planet reference	\$	C	Prbit velocity vector	
	?			
Pointing vector	₩₽	Po	pinting vector	
X 1		x	0	
YO		Y	0	
ZO		z	1	
OrbitCenter or anti-OrbitCenter				
Orbit planet reference	\$			
VARIABLES				
Please use "Edit Variables" 🗙 ?				

Figure 5 - Kinematics - Simple Case

2.4 Mission

Now that the model, the meshing, the trajectory and the attitude are defined, they all can be joined together in the mission tab. Please refer to the Systema User Manual to have more information on the mission definition.

2.5 Processing

All is ready to setup the final computation parameters and to launch the computation. To create an Atomox computation, select the Atomox module, drag and drop it in the processing middle window.

simple_case.sysprc *	
Current Mission Mission data Atomox	H5 Log Out

Figure 6 - Processing - Simple Case - Process parameters

The Atomox computation module presents itself like in the figure above. On the left of the box is the file needed as input for the computation. It is generated by default from Systema. Once the computation is done, the output file on the right on the box are generated.





Output files

- The H5 file, which is the binary file, contains all the computational data, per time step and per node. It can be read with a H5 reader, or directly in Systema with the graph function and the results display in the meshing. The process will be detailed later on in this guide. The data available in the H5 are:
 - Absorbed Fluence (/cm2)
 - Absorbed Flux (/cm2/s)
 - Direct Fluence (/cm2)
 - Direct Flux (/cm2/s)
 - Total Fluence (/cm2)
 - o Total Flux (/cm2/s)
 - Erosion (µm)
 - Equivalent Angle (deg) (angle taken between the normal of the mesh and the velocity direction)
 - Average Velocity (m/s)
 - Normal Impact Energy (eV)
- The Log file, which gives information on the computation status. Some other data such as the atmospheric values generated by Atomox are displayed.
- The Out File, which is a text file. The figure below gives an example of an out file.





ŧ,	****	*****	******	*****	*******	****	******	***
ŧ								4
ŧ		Atomic	Oxygen	Flux	computed	by	Atomox	1
ŧ								4
÷,	****	******	******	*****	*******	****	******	***

\$INFOS

#

#

File : Assemblage version	3.atx.out	
Executed on : Wed Mar 08	15:53:23 2023	
Input files :		
- Sysset : Assemblage ve	ersion 3.sysset	
Parameters :	-	
- Random seed : 876743		
- Ray emission (high cr:	iticity) :	
- Number of rays per	radiative mesh	: 20
- Ray emission (normal o	criticity) :	
- Number of rays per	thermal node :	200
- Ray emission (low crit	ticity) :	
- Number of rays per	thermal node :	200
- Ray threshold : 1%		
- Thermal Velocity:	OFF	
- Wind Velocity:	OFF	
- MultiReflections:	ON	
- Maximum Reflections :	200	
Entiretien should.	1 00	

- F10.7 Solar activity: 50.00 - AP Magnetic index : 10.00

ŧ					h	fax '	values of						
ŧ	Time	1	O Density	1	Velocity	1	V*No Flux	1	Direct Flux	1	Total Flux	1	Tot Fluence
ŧ	(5)	1	(/cm3)	1	(m/s)	1	(/cm2/s)	1	(/cm2/s)	1	(/cm2/s)	1	(/cm2)
٤.	0.00e+000	1	9.45e+001	1	7.35e+003	1	6.94e+007	1	6.94e+007	1	7.05e+007	1	0.00e+000
	7.00e+002	1	1.61e+001	1	7.35e+003	1	1.18e+007	1	1.18e+007	1	1.20e+007	1	2.89e+010
	1.40e+003	1	3.96e+000	1	7.35e+003	1	2.91e+006	1	2.91e+006	1	2.96e+006	1	3.41e+010
	2.10e+003	1	4.23e+000	1	7.35e+003	1	3.11e+006	1	3.11e+006	1	3.15e+006	1	3.62e+010
	2.80e+003	1	2.08e+000	1	7.35e+003	1	1.53e+006	1	1.53e+006	1	1.55e+006	1	3.79e+010
	3.50e+003	1	2.35e+000	1	7.35e+003	1	1.73e+006	1	1.73e+006	1	1.75e+006	1	3.90e+010
	4.20e+003	1	1.55e+001	1	7.35e+003	1	1.14e+007	1	1.14e+007	1	1.15e+007	1	4.37e+010
	4.90e+003	1	5.92e+001	1	7.35e+003	1	4.35e+007	1	4.35e+007	1	4.42e+007	1	6.32e+010
	5.60e+003	1	1.21e+002	1	7.35e+003	1	8.89e+007	1	8.89e+007	1	9.02e+007	1	1.10e+011
	6.30e+003	1	9.45e+001	1	7.35e+003	1	6.94e+007	1	6.94e+007	1	7.05e+007	1	1.66e+011

ŧ	Results for group All									
# Positive Side										4
1	Time	1	Direct Flux	1	Total Flux	1	Tot Fluence	1	Mean erosion	
ŧ	(5)	1	(/cm2/s)	1	(/cm2/s)	1	(/cm2)	1	(um)	
	0.00e+000	1	1.06e+007	1	2.78e+007	1	0.00e+000	1	0.00e+000	
	7.00e+002	1	1.79e+006	1	4.73e+006	1	1.14e+010	1	1.14e-014	
	1.40e+003	1	4.42e+005	1	1.17e+006	1	1.35e+010	1	1.35e-014	
	2.10e+003	1	4.72e+005	1	1.25e+006	1	1.43e+010	1	1.43e-014	
	2.80e+003	1	2.33e+005	1	6.13e+005	1	1.50e+010	1	1.50e-014	
	3.50e+003	1	2.62e+005	1	6.91e+005	1	1.54e+010	1	1.54e-014	
	4.20e+003	1	1.73e+006	1	4.55e+006	1	1.72e+010	1	1.72e-014	
	4.90e+003	1	6.61e+006	1	1.74e+007	1	2.49e+010	1	2.49e-014	
	5.60e+003	1	1.35e+007	1	3.56e+007	1	4.35e+010	1	4.35e-014	
	6.30e+003	1	1.06e+007	1	2.78e+007	1	6.57e+010	1	6.57e-014	

Figure 7 - Processing - Simple Case - Out file.txt

- The content of the file is some computational parameters, the max results of all shapes of the computation. The data that is presented is the time of computation, the atomic oxygen density, the ATOX flux computed as the ATOX density * the spacecraft velocity, the Direct Flux (no reflection taken into account), the total flux (direct flux + reflections) and the total fluence (integration of the total flux over time).
- The following tables contain the results on the groups, for all the positive sides and all the negative sides. The user has to make sure all his surface of interest in a group are on the same side otherwise results may be difficult to interpret. The results are the average over all active





positive or negative sides of surfaces in the group.

- The Rays file, a binary file that contains the rays used for the computation. This is deactivated per default as the generated file can be quite big. It can be activated by right clicking on the bullet and activate. The rays can be displayed in the meshing tab. The process is described later in the documentation.

Computational parameters

When clicking on the Atomox module, the computation parameters are displayed. In the Atomox tab, two sub-tabs are available: the atmosphere parameters tab that allow specifications for the proper computation of Thermal and Wind velocity, and the Ray Tracing tab that specify computational options with regard to the ray tracing settings.

Atomox Common Gen	eral
RUN PARAMETERS	Revert
Atmosphere parameters	Ray Tracing
Thermal Velocity	
On	\$
Atmosphere Model	
Generate Table (NRL-MSIS	00) 🗘
Wind Velocity	
On	\$
Wind Model	
Generate Table (HWM07)	\$
Ар	₩
15	
F10.7	₩
150	10E-22 W/m2/Hz

Figure 8 - Atmosphere Parameters

The Atmosphere parameters are the following:

- Thermal Velocity: ON or OFF option. If on, the thermal velocity will be taken into account for the computation, and will affect the ray direction. More details are available in the Theoretical Background section.
- Atmosphere Model: It is possible to choose between the NRL-MSIS00 model or a basic model where the atomic oxygen density and the temperature are constant and user-defined.
- Wind Velocity: ON or OFF option. If on, the wind velocity will be taken into account for the computation, and will affect the ray direction. The option is available for the NRL-MSIS00 atmosphere model only. More details are available in the Theoretical Background section.
- Wind Model: fow now, only the HWM07 model is available.



• Ap: Earth magnetic index, which is an input for the NRL-MSIS00 and the HWM07 models.

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• F10.7: At the same time is the daily F10.7 and the 3 month average D10.7 solar flux (10^{-22} W/m²/Hz), it is an input for the NRL-MSIS00 and the HWM07 models.

The Ray tracing parameters are the following:

tomox Common	
RUN PARAMETERS	Revert
Atmosphere parameters Ray Tracing	
Method	
Monte-Carlo	\$
Random seed	₩
876743	
Multiple reflections	
Yes	\$
Ray threshold	₩
1	%
Extinction Factor/Maximum ray bounces	₩
10	
Critical Ray building method	
Per node	+
Critical Ray number per node	₩
20000	
Ray building method	
Per node	÷
Ray number per node	₩
2000	
Low Ray building method	
Per node	\$
Low Ray number per node	₩

Figure 9 - Ray tracing parameters

- Method: Ray tracing algorithm, only Monte-Carlo is available for now.
- Random seed: random seed for random matrix
- Multiple reflections: Yes or No. Yes allows the multiple reflections, and No stop the ray at first impact. If Yes is selected, the following options are available:
 - Ray threshold: Percentage of energy towards which the ray is considered to stop.
 - o Extinction Factor: Give maximum number of reflections possible for a ray.
- Critical Ray building method: Choice to setup number of ray for the Critical tag (setup in the modeler) per Node, Mesh or Density
- Critical Ray number per node: Number of rays fired per Node, Mesh or Density.
- Ray building method: Choice to setup number of ray for the Normal tag (setup in the modeler) per Node, Mesh or Density
- Ray number per node: Number of rays fired per Node, Mesh or Density.





- Low Ray building method: Choice to setup number of ray for the Low tag (setup in the modeler) per Node, Mesh or Density
- Low Ray number per node: Number of rays fired per Node, Mesh or Density.

Once all these parameters are setup, the user can launch the computation, clicking on

2.6 Post-Processing

In order to post-process the results, the user can look in the atx.log file and the .out file to check mean values. Another way to get results from the simulation is to use the post-process tab, and convert h5 files into csv files. More detail on that is available in the Systema User Manual.

For the purpose of closing this getting started, the data will be here displayed in the 3D view.

To generate such images and results, once the computation is completed, the user can go in the Modeler/meshing tab. Then, clicking in the configuration window.

3D View (1)_2 configura	ition	×
Entities configuration Display Orientation Information Color Video recording	Entities configuration simple_case.sysmsh Shape Appearance Textual information Shape orientation Numbering identifiers Result simple_case_simple_case simple_case.atx.h5 Absorbed Fluence (/cm2) Absorbed Fluence (/cm2) Direct Fluence (/cm2) Direct Fluence (/cm2) Direct Fluence (/cm2) Direct Fluence (/cm2) Total Fluence (/cm2) Configure	Unload Rays display
		Close

Figure 10 - Post-Processing - Simple Case - Configuration window

The user can select in the Shape Appearance, in the Results/.../simple_case.atx.h5 the data to be displayed in colour mapped on the model. Textual information can be also selected to get accurate data on a specific





node. Finally the Rays display can be used if activated during the computation. This allows to check the particles passing during the computation.



Figure 11 - Post-Processing - Simple Case - Ray Display

3 Theoretical background

3.1 Physical Modeling

3.1.1 Introduction

The final goal of an atomic oxygen analysis is to assess the fluence of atmospheric particles to outer surfaces of a spacecraft. Resulting material erosion is taken as proportional to the fluence of particles on this surface.

The fluence, is by definition, the integration over time of the flux crossing this surface. The flux on a totally exposed surface (ram flux) is the product of the particle number density by the average velocity of the particle.

Consequently, density and velocity are the first quantities to study. Densities are given by different atmosphere models. These models are used by the software as external tools. Velocity computation is developed in the following section.

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3.1.2 Velocity Computation

The velocity of a molecule is the sum of the aerodynamic velocity and the thermal motion. For the computation of the thermal motion, the Maxwellian theory of gas dynamics is used. In particular, this theory assumes an isotropic distribution. The velocity \vec{v} is given by:

$$\vec{\mathbf{v}} = \vec{\mathbf{v}}_{\text{aero}} + \vec{\mathbf{u}} \,, \tag{1}$$

where:

 \vec{u} : Thermal motion vector.

 \vec{v}_{aero} : Aerodynamic velocity vector.

The thermal motion \vec{u} is such that its components follow a normal distribution with probability density f given by:

$$f(u_i) = \frac{1}{\sqrt{\pi} u_m} \exp\left(-\frac{u_i^2}{u_m^2}\right), \qquad (2)$$

with:

 u_{m} : Thermal velocity.

 u_i : x, y or z coordinate of thermal motion.

The thermal velocity u_m is defined by:

$$u_{\rm m} = \sqrt{\frac{2RT}{M}} , \qquad (3)$$

with:

T: ambient temperature (K).

R: universal gas constant (314 J/kmol/K).

M: molecular weight (kg/kmol).

The aerodynamic velocity is the difference between the wind velocity vector and the spacecraft velocity vector:

$$\vec{\mathbf{v}}_{\text{aero}} = \vec{\mathbf{v}}_{\text{w}} - \vec{\mathbf{v}}_{\text{S/C}}, \qquad (4)$$

where:

 $\vec{v}_{\rm w}$: Wind velocity in inertial frame determined using a wind model.

 $\vec{v}_{s/c}$: Spacecraft velocity in inertial frame.

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3.1.3 Flux Computation

The flux Φ of oxygen atoms (particles/cm2/sec) impacting a given surface assumed to be totally exposed is equal to the product of the local atomic oxygen number density (particles/cm3) by the average velocity (cm/sec) of particles impacting this surface.

For instance, if we assume that the inward surface normal gives the direction of the x-axis, one has to calculate the average velocity on x of particles having vx>0.

This average velocity is given by:



Figure 12 - Velocity impacting a surface

$$\overline{\mathbf{v}}_{\mathrm{x}} = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \mathbf{v}_{\mathrm{x}} f(\vec{\mathbf{v}} - \vec{\mathbf{v}}_{\mathrm{aero}}) d\mathbf{v}_{\mathrm{x}} d\mathbf{v}_{\mathrm{y}} d\mathbf{v}_{\mathrm{z}}, \qquad (5)$$

and the flux Φ is computed as $\Phi = N_0 \overline{v}_x$, where N0 is the number density of oxygen atoms. Completing the integration in the above equation yields:

$$\Phi = N_0 \sqrt{\frac{RT}{2\pi M}} \left[e^{-s^2} + \sqrt{\pi} s \left(1 + \operatorname{erf} \left(s \right) \right) \right], \tag{6}$$

with:

s: molecular speed ratio.

erf: error function.

The molecular speed ratio s is given by:

$$s = \frac{\vec{v}_{aero}.\vec{x}}{u_m},$$
(7)

and the standard error function erf is defined by:

$$\operatorname{erf}(s) = \frac{2}{\sqrt{\pi}} \int_{0}^{s} e^{-x^{2}} dx.$$
 (8)

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3.1.4 Shadowing Analysis

3.1.4.1 Apparent surface

The method exposed on previous sections to compute velocity and flux is adequate if the surface is totally exposed to the incident flux. In a 3D geometrical model, some surfaces may be totally exposed, some surfaces can be half shadowed, and some surfaces can be totally masked.

The flux will now be the product of the previous flux by the percentage of apparent surface.

The ray-tracing is very well adapted to compute the percentage of apparent surface. If we fire a great number of rays from an element (triangle of quadrangle), in the opposite direction of particles velocity, the percentage of apparent surface A is:

$$A = \frac{\sum_{i \in J} WG_i}{\sum_{i=1}^{N_i} WG_i},$$
(9)

where:

J: {i / ray i hits the surface}. Nt: total number of emitted rays. WGi: weight of ray i.

For a triangle, the weight WG of a ray is always 1, and for a quadrangle, the weight depends on the sampled point.

3.1.4.2 Velocity direction

To fire rays, we must know the emission direction, i.e. the particle velocity direction. Note that we are interested in the direction of particles, only for emitting rays and computing the percentage of apparent surface, not for computing the flux, as it is already known.

From each sampled point, a direction \vec{v} is determined such that:

$$\vec{\mathbf{v}}.\vec{\mathbf{x}} > 0, \tag{10}$$

where:

 \vec{x} : surface inner normal.

 \vec{v} : particle velocity vector.

(which is the condition for \vec{V} to reach the surface).

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This relation can also be written as:

$$\mathbf{u}_{\mathrm{x}} > -\vec{\mathbf{v}}_{\mathrm{aero}} \cdot \vec{\mathbf{x}} \,, \tag{11}$$

where ux is the x coordinate of thermal motion vector.

Only the thermal motion has to be sampled at random. Thus, to obtain a random velocity, three numbers,

 $\chi_{\rm x}$, $\chi_{\rm y}$ and $\chi_{\rm z}$ are selected at random in the [0,1] interval such that:

$$\chi_{x} = \frac{\int_{-\vec{v}_{aero},\vec{x}}^{u_{x}} f(u) du}{\int_{-\vec{v}_{aero},\vec{x}}^{\infty} f(u) du} > -\vec{v}_{aero}, \vec{x}, \qquad (12)$$

$$\chi_{y} = \int_{-\infty}^{u_{y}} f(u) du , \qquad (13)$$

$$\chi_z = \int_{-\infty}^{u_z} f(u) du , \qquad (14)$$

where f is given by equation (3).

After integration we obtain:

$$\chi_{x} = \frac{\operatorname{erf}\left(\frac{u_{x}}{u_{m}}\right) + \operatorname{erf}\left(S_{x}\right)}{1 + \operatorname{erf}\left(S_{x}\right)},$$
(15)

$$\chi_{\rm y} = \frac{\operatorname{erf}\left(\frac{u_{\rm y}}{u_{\rm m}}\right) + 1}{2}, \qquad (16)$$

$$\chi_{z} = \frac{\operatorname{erf}\left(\frac{u_{z}}{u_{m}}\right) + 1}{2}, \qquad (17)$$

where Sx is given by:

$$S_{x} = \frac{\vec{v}_{aero} \cdot \vec{x}}{u_{m}} \,. \tag{18}$$





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These equations are inverted to give the coordinates of the thermal motion vector:

$$u_{x} = u_{m} \operatorname{erf}^{-1}((\chi_{x} - 1) \operatorname{erf}(S_{x}) + \chi_{x}), \qquad (19)$$

$$u_{y} = u_{m} \operatorname{erf}^{-1}(2\chi_{y} - 1),$$
 (20)

$$u_z = u_m \operatorname{erf}^{-1}(2\chi_z - 1).$$
 (21)





3.1.5 Multiple Reflections

3.1.5.1 Theoretical background

The impingement of molecules on surfaces is a physical phenomenon difficult to model since, up to now, few experiments exist on this subject.

The features considered in the present reflection model are the following:

- The direction of the reflected particles, which depends on the surface material, and on the angle of impingement,
- The velocity of the reflected particles, which depends on the surface material, and on the velocity of impingement.

In order to model these features, three coefficients are defined for each material:

 Ω : absorption coefficient, is the percentage of flux absorbed by the material.

Sr: specularity coefficient, is the percentage of flux reemitted specularly by the material.

Dr: Diffuse reflection coefficient, is the percentage of flux reemitted specularly by the material.

r: accommodation ratio, is the coefficient applied to re-emission velocity modulus, in the case of diffuse reflection.

The absorption, specularity and diffuse reflection coefficient are related by the following relationships:

$$\Omega + \rho_{\rm s} + \rho_{\rm d} = 1, \qquad (22)$$

with:

 ho_{s} : specular reflection coefficient, is the percentage of flux specularily reflected.

 $\rho_{\rm d}$: diffuse reflection coefficient, is the percentage of flux diffusely reflected.





3.1.5.2 Method

The ray-tracing technique is very well adapted for treating multiple-reflection especially because it has already been used to compute the first impact. The method is the following.

We start from a ray carrying a certain number of particles, say N:

- Part of this number is absorbed by the surface. The number of absorbed particles $\,{}^{N_a}$ is $\,{}^{\Omega N}$.
- Part of this number is specularly reflected. The reflection angle is equal to the incident angle. The number of specularly reflected particles from its point of impact N_s is $\rho_s N$.

The ray is re-emitted:

- If the ray strikes no surface, the ray stops, the secondary flux is set to zero.
- If the ray strikes a surface, the process of absorption-reflection starts again for the ray and the hit surface. The process stops when the remaining flux is smaller than a user defined percentage of the first impact flux, or when the number of reflections is greater than a user defined maximum number of reflections.
- Part of this number is diffusely reflected in a user defined number of rays M, following Lambert's law. In the V3 Atomox version, M was a user coefficient to setup. In the V4 version current version, this is

set per default to 1. Each diffusely reflected ray carries a number of particles N_d given by:

$$N_{d} = \frac{\rho_{d} N}{M} (1 - r), \qquad (23)$$

- The rays are re-emitted from the point of impact:
 - The flux of the rays striking a surface is transferred to this surface.
 - The flux of the rays striking no surface is lost.
 - In any case, the rays stop.





3.1.6 Spin

The ATOMOX software is able to consider the case of a spinning satellite. In this case, the user defines:

- The spin axis vector,
- The number N of positions around the spin axis to be accounted for in the analysis.

The method is the following:

- Rays are fired for the first spin position providing the incoming flux for this spin position (the first spin position is defined in the POINTING module). The rotation of the satellite is then performed by a rotation of the satellite velocity vector around the spin axis vector in the Satellite Reference Frame. The rotation angle is 2π/N where N is the number of spin positions (user defined). This step is repeated N-1 times.
- After N rotations, the flux is averaged over the number of positions.

This method is time-consuming, time being proportional to the number of spin positions.







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$$\vec{d}_{1} = \begin{vmatrix} d\sin\theta\cos(\varphi_{1}) \\ d\sin\theta\sin(\varphi_{1}), \\ d\cos\theta \end{vmatrix}$$
(24)

$$\vec{d}_{i} = \begin{vmatrix} d\sin\theta\cos\left(\phi_{1} + (i-1)\frac{2\pi}{N}\right) \\ d\sin\theta\sin\left(\phi_{1} + (i-1)\frac{2\pi}{N}\right) \\ d\cos\theta \end{vmatrix},$$
(25)

where:

 \vec{d}_1 : ray direction.

N: number of spin positions.

- \vec{d}_i : ith ray direction.
- \vec{n} : spin axis vector.

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3.1.7 Fluence Computation

As already stated in the introduction, fluence is, by definition, the integration over time of the flux crossing a surface.

Fluence can also be defined as the product of the average flux, during a certain time, by this time. As flux is computed on a discretised number of times, (the orbital positions), this definition is used in the ATOMOX software.

A recurrent method of trapezes is used. The fluence Φ_i at orbital position i is given by the following relationships:

$$\Phi_1 = 0,$$
 (26)

$$\Phi_{i} = \Phi_{i-1} + \frac{\phi_{i} + \phi_{i-1}}{2} (t_{i} - t_{i-1}), \qquad (27)$$

where:

 Φ_i : flux at orbital position i.

ti: Julian date at orbital position i.

3.2 Atmosphere Models: Inputs and Outputs

3.2.1 The NRLMSISE-00 atmosphere model

The NRL Mass Spectrometer, Incoherent Scatter Radar Extended Model (NRLMSISE-00) model describes the neutral temperature and species densities in Earth's atmosphere. It is based on a very large underlying set of supporting data from satellites, rockets and radars, with extensive temporal and spatial distribution. It has been extensively tested by the global scientific community against experimental data. The model has a flexible mathematical formulation. It is valid for use from ground level to the exosphere. The Mass Spectrometer and Incoherent Scatter (MSIS) series of models developed between 1977 and 1990 are used extensively by the scientific community for their superior description of neutral composition. The models utilized atmospheric composition data from instrumented satellites and temperatures from ground-based radars. The initial MSIS 1977 model was based on the Jacchia temperature profile framework, but the density at 120 km varied with local time and other geophysical parameters to fit the measurements. Exospheric temperature and density variations were represented by spherical harmonics resulting in requiring fewer parameters for a given level of accuracy. Subsequent versions of the model include the longitude variations, a refined geomagnetic storm effect, improved high latitude, high solar flux data and a boundary lowered to sea level. The NRLMSISE-00 model of atmospheric composition, temperature, and total mass density from ground to exobase includes the following:

- Drag data based on orbit determination
- More recent accelerometer data sets
- New temperature data derived from Millstone Hill and Arecibo incoherent scatter radar observations





• Observations of O2 by the Solar Maximum Mission (SMM), based on solar ultraviolet occultation.

A new species, "anomalous oxygen," primarily for drag estimation, allows for appreciable O+.

For this model, the following parameters are used.

Input parameters:

Year and day in the year (YYDDD) Seconds in the day (UT seconds) Altitude (kilometres) (range: > 85 km) Latitude (degrees) Local solar time (decimal hours) Daily F10.7 solar flux (10⁻²² W/m²/Hz) 3 month average F10.7 solar flux (10⁻²² W/m²/Hz) Magnetic index (Ap) Mass number of the selected species

Output parameters:

Helium number density (/cm³) Atomic oxygen number density (/cm³) Molecular nitrogen number density (/cm³) Molecular oxygen number density (/cm³) Argon number density (/cm³) Atomic hydrogen number density (/cm³) Atomic nitrogen number density (/cm³) Total density (g/cm³) Exospheric temperature (K) Temperature at altitude (K)





3.2.2 The HWM07 Horizontal Wind Model 2007

HWM07 is an empirical model of horizontal winds in the troposphere, stratosphere, mesosphere, and thermosphere, and is intended to succeed HWM93 [Hedin et al., J. Atmos. Terr. Phys., vol. 58, 1421-1447, 1996]. In addition to the data used in HWM93, the model is based on extensive new ground-based and space-based wind measurements, including height profiles from NASA-UARS/WINDII, NASA-UARS/HRDI, measurements from ground-based optical and radar instruments obtained from the NSF-CEDAR database, and lower atmospheric NCEP data.

In the thermosphere, the model consists of two parts: a quiet-time portion, and a geomagnetically disturbed portion. The quiet-time part represents average wind conditions when ap <= 12. The disturbed part represents average perturbation winds for the specified ap input.

The quiet part is represented by vector spherical harmonics in geodetic latitude, geodetic longitude, and solar local time, up to wave number 8 in latitude, 2 in longitude, and 3 in local time. The seasonal dependence is represented by harmonic terms up to semiannual. The vertical structure is represented below 250 km by cubic B-splines with node spacing of 5 km below 110 km and higher nodes at 110, 117, 125, 135, 150, 200, and 250 km. Above 250 km, an exponential decay function with a scale height of 60 km is used; continuity up to the second derivative is imposed at 250 km.

The disturbance winds depend on magnetic latitude, magnetic local time, and Kp. The Quasi-Dipole magnetic coordinates described by Richmond [J Geomagn. Geoelectr., vol. 47, 191-212, 1995] are used for the magnetic coordinates; the code was obtained from the NSF-CEDAR database, and the interpolation grid was computed from IGRF at 250 km and epoch 1994.0 (a modified FORTRAN-90 version of the code, apexcord.f90, is included in this package; it contains only those subroutines needed for reading the interpolation grid and computing QD coordinates). The magnetic latitude and magnetic local time dependence of the disturbance winds is represented by vector spherical harmonics up to wave number 10 in magnetic latitude and wave number 3 in magnetic local time. At mid and low latitudes, only latitudinal terms up to wave number 4 are used; the transition from low resolution at low latitudes to high resolution at high latitudes occurs at a pre-determined latitude that depends on local time and Kp. The transition is made with an exponential function with a width of 4 degrees. The Kp dependence is represented by cubic splines with nodes at 0, 2, 5, and 8. The Kp dependence is constrained to have zero slope at Kp=0 and Kp=8, and is constant above Kp=8.

Input parameters:

Year and day (YYDDD) Seconds in the day (UT seconds) Altitude (kilometres) (range: 100 – 850 km) Latitude (degrees) Longitude (degrees) Local solar time (decimal hours) Daily F10.7 solar flux (10⁻²² W/m²/Hz) 3 month average F10.7 solar flux (10⁻²² W/m²/Hz) Magnetic index (Ap)

Output parameters:

Meridional wind (northward) (m/s) Zonal wind (eastward) (m/s)