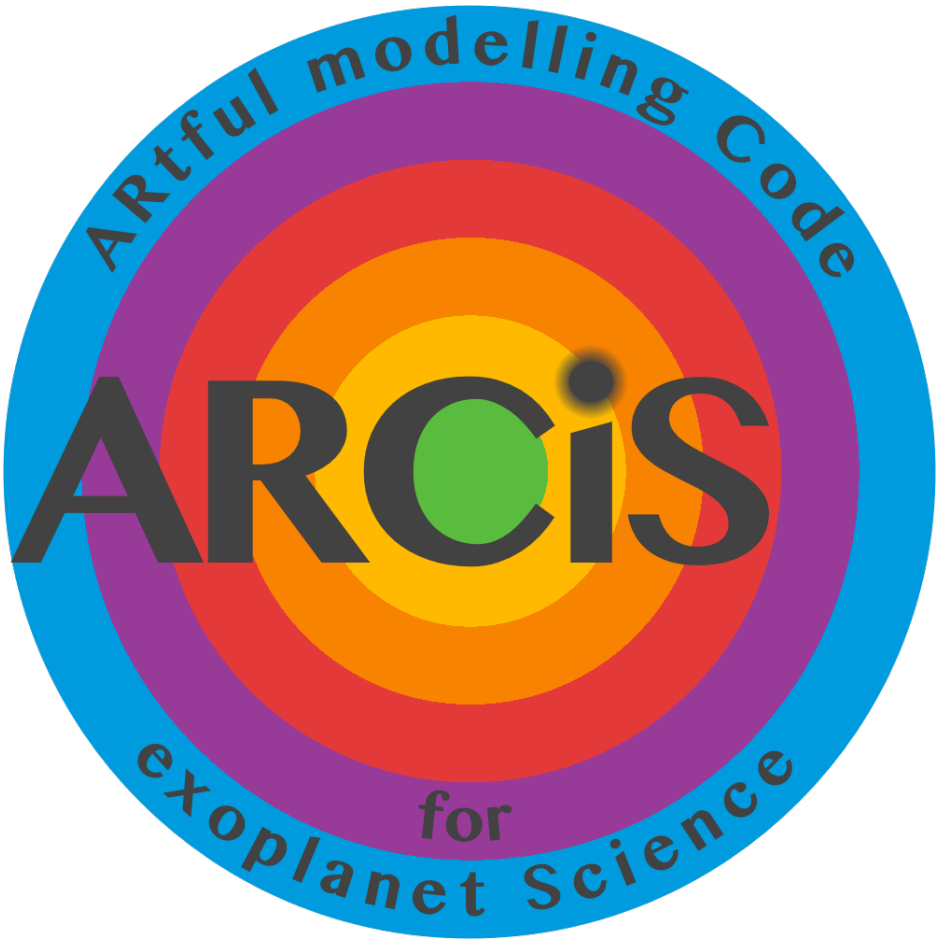

User Guide to ARCiS

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1 Introduction

1.1 Terms of use

By using ARCiS you agree to the following:

- If in doubt on any of the results, you consult with me. Email: M.Min@sron.nl
- You cite the appropriate papers listed below.

The most important reason for this is to make sure that ARCiS is used in a correct way and the result are scientifically useful. ARCiS is a complex code which can do a lot of things, this also means things can go wrong. Please refer to Min et al. [2020] for the first full description of the fundamental properties of the code.

Note that there are several parts of the code from different developers:

- Cloud formation framework: Ormel and Min [2019]
- Optical properties of cloud particles computed using DHS: Min et al. [2005], Toon and Ackerman [1981]
- Refractive indices for the cloud species, see references in Min et al. [2020]
- Molecular opacities: Chubb et al. [2021] and references therein
- Multinest Retrieval tools: Feroz and Hobson [2008], Feroz et al. [2009, 2019]
- GGchem when including chemistry: Woitke et al. [2018]
- Disequilibrium chemistry implementation: Kawashima and Min [2021]
- Diffusion implementation for 3D structures: Chubb and Min [2022]
- Coupling with planet formation parameters: Khorshid et al. [2022]

2 Installing ARCiS

Before installing ARCiS you need:

A Fortran compiler: This can be either `gfortran` or `ifort` (any other might work but is not tested).

`cfitsio` library: This is needed to allow fortran to read and write binary fits files.

`MultiNest`: This allows ARCiS to perform Bayesian retrievals.

On a Mac the easiest is to install cfitsio through HomeBrew (google 'homebrew' for installation instructions. After that:

```
# brew install cfitsio
```

Next fetch MultiNest:

```
# git clone https://github.com/JohannesBuchner/MultiNest.git
# cd MultiNest/build
# cmake ..
# make
# sudo make install
```

Next fetch the git source code from:

```
# mkdir ARCiS ; cd ARCiS
# git clone https://github.com/michielmin/ARCiS.git ./src
# cd src
# make gfort=true multi=true
```

This creates the ARCiS binary, which you can put in any path accessible (/usr/bin or something like that).

You also need data files to be stored under: `$(HOME)/ARCiS/Data/`
These data files can be downloaded from http://www.exoclouds.com using the password: ARCiSData

3 Using ARCiS

To run ARCiS you further only need an input file. On the prompt type:

```
# ARCiS inputfile.dat -o outputdir
```

which creates the output directory `outputdir` containing the output files.

There are several options included in ARCiS. These are given as keywords in the `inputfile.dat` file (or whatever you call it). Keywords are always given as `key=value` and can be anywhere in the file (order does not matter). Also, you can overwrite keywords set in the input file from the command line in the following way

```
# ARCiS inputfile.dat -o outputdir -s key1=value1
```

Any number of keys can be set on the command line. Just make sure the first argument of the command line is the name of your input file. Note that ARCiS always takes the last keyword value it encounters, first reading the input file, next the command line keywords one by one.

4 Keywords

There are many keywords for a variety of different setups. Chemistry or not, cloud formation or not, various temperature structures, perform retrievals, 3D or 1D structure, and many more options. Below are some very basic setups discussed. The runtime of a single forward model can vary from 0.01 second to 15 minutes depending on your choices. For more information it is best to get in contact.

4.1 Base properties

`Rp` Radius of the planet in Jupiter radii.

`Mp` Mass of the planet in Jupiter masses.

`Pp` Atmospheric pressure corresponding to radius `Rp`. Default is 10 bar.

`Tstar` Temperature of the host star in K.

`Rstar` Radius of the host star in Solar radii.

`distance` distance to the system in parsec.

`Dplanet` Distance of the planet to the star in AU.

planetname Name of the planet to read from the database. Radius, mass and distance of the planet and the star are read from the database.

4.2 Grid setup

pmin, pmax Minimum, maximum pressure considered in the atmosphere

nr Number of pressure points

lmin, lmax Minimum, maximum wavelength considered in micron. Note that for temperature computations these must be set wide enough to ensure energy balance is properly computed.

specres Spectral resolution R in lambda/dlambda

specresdust Spectral resolution for computation of the solid state species in the clouds.

4.3 Abundances of the molecules

Homogeneous abundances can be set using keywords like e.g. `H2O=1d-4`. Only molecules that are defined through this somewhere in the input file are taken into account. These abundances are overwritten when chemistry is used.

chemistry Logical determining if chemistry is computed or not (either .true. or .false.)

condensates Logical determining if condensates should be taken into account in the chemistry computations (default is .false. and most stable is to leave it like that).

COratio C/O ratio of the atmosphere

metallicity Metallicity of the atmosphere

4.4 Opacities and raytracing

cia Logical determining if CIA is taken into account

maxtau Maximum optical depth considered for the raytracing

compute Logical determining if the opacities need to be recomputed from the linelists

scattering Logical determining if scattering of the thermal radiation is included

scattstar Logical deternining if scattering from the star is included

4.5 Temperature structure

computeT Logical determining if the temperature structure is computed self-consistently

maxiter Maximum number of iterations for the temperature structure

betaT Cosine of the angle of incoming radiation.

TeffP Effective temperature of the radiation from inside the planet

Tp Temperature of the planet at 1 bar when `computeT=.false.`

dTp Temperature gradient when `computeT=.false.`

$$\log_{10}(T[\mathrm{K}]) = \log_{10}(T_p[\mathrm{K}]) + dT_p \log_{10}(P[\mathrm{bar}]) \tag{1}$$

4.6 Other options

4.6.1 K_{zz} setup

The diffusion of the atmosphere is important for the disequilibrium chemistry and for the cloud formation. For the clouds it is possible to set a separate homogeneous value or use the global defined K_{zz} profile. The disequilibrium chemistry always uses the globally defined K_{zz} profile.

Two cases are considered:
when $K_{zz}^{contrast} > 1$:

$$K_{zz} = \max\left[K_{zz}^{deep}; \min\left[\left(K_{zz}^{deep} \cdot K_{zz}^{contrast}\right); \left(K_{zz}^{1bar} P^{-|\gamma_K|}\right)\right]\right] \tag{2}$$

when $K_{zz}^{contrast} < 1$:

$$K_{zz} = \max\left[\left(K_{zz}^{deep} \cdot K_{zz}^{contrast}\right); \min\left[K_{zz}^{deep}; \left(K_{zz}^{1bar} P^{|\gamma_K|}\right)\right]\right] \tag{3}$$

This profile is used when K_{zz}^{deep} and K_{zz}^{1bar} are defined. By default these are set to negative values, which means the homogeneous value for K_{zz} is used.

Keywords:

Kzz Sets the value used for homogeneous global K_{zz}

Kzz_deep Sets the value used for K_{zz}^{deep}

Kzz_1bar Sets the value used for K_{zz}^{1bar}

Kzz_contrast Sets the value used for $K_{zz}^{contrast}$

Kzz_p Sets the value of γ_K (default is 0.5)

4.6.2 Photochemical reactions

There is the option to simulate photochemical reactions in ARCiS. This is done by converting molecules or atoms above a certain optical depth in the atmosphere into other molecules or hazes. The conversion efficiency of the reaction is parameterised by the simple equation

$$f_{\text{conversion}} = f_{\text{eff}}\, e^{-\tau_{\text{UV}}}, \tag{4}$$

Here τ_{UV} is simply computed from the parameter κ_{UV} that can be given as an input parameter. The global efficiency f_{eff} determines the maximum efficiency possible. Note that $f_{\text{conversion}}$ is capped at 1 in the code. So it is possible to give $f_{\text{eff}} > 1$, but this will only result in an efficiency that is equal to 1 up to lower pressures.

The global keyword is:

kappaUV Sets the value used for κ_{UV}

The rest is set per reaction.

As an example, consider we want to convert sulfur and oxygen into SO2

$$\text{S} + 2\,\text{O} \rightarrow \text{SO}_2 \tag{5}$$

This is done by setting

photoreac1:S=1 Sets the reactant of reaction 1 to contain 1 S atom

photoreac1:O=2 Sets the reactant of reaction 1 to contain 2 O atoms

photoprod1:SO2=1 Sets the product of reaction 1 to contain 1 SO_2 molecule

Converting atoms to molecules is done before chemical calculations (so the atoms are removed from the atomic mixture and the molecular products are added later on)

We can also convert for example

$$H_2S + 2\,H_2O \rightarrow SO_2 + 3\,H_2 \tag{6}$$

This is done by setting

photoreac1:H2S=1 Sets the reactant of reaction 1 to contain 1 H2S molecule

photoreac1:H2O=2 Sets the reactant of reaction 1 to contain 2 H2O molecules

photoprod1:SO2=1 Sets the product of reaction 1 to contain 1 SO_2 molecule

photoprod1:H2=3 Sets the product of reaction 1 to contain 3 H_2 molecules

Converting molecules into other molecules is done after the chemical computations (so first it is determined how much H_2S and H_2O would be available.

To produce haze, e.g. the reaction

$$CH_4 \rightarrow \text{haze} \tag{7}$$

This is done by setting

photoreac1:CH4=1 Sets the reactant of reaction 1 to contain 1 CH4 molecule

photohaze1=1 Sets the product of reaction 1 to be haze particles with 1 C atom per converted CH4 molecule

Finally the keyword

photoeff1 sets the value for $f_{\rm eff}$ of the reaction

4.7 Retrieval

4.7.1 Observations

obs1:type Can be ”trans”, ”emis” or ”emisR”.

obs1:file Filename with the observation. Should be in format:
column1: wavelength in micron
column2: trans or emis spectrum (same units as the output file to compare with)
column3: error
column4: spectral resolution of this wavelength bin (so $\lambda/\Delta\lambda$)

obs1:beta Weight of this observation. Only relevant if more than one obs is defined.

4.7.2 Parameters

fitpar:keyword Keyword to be retrieved. This key switches automatically to the next retrieval parameter.

fitpar:min Minimum value considered

fitpar:max Maximum value considered

fitpar:log Logical determining if the parameter is sampled logarithmically

4.8 Very rough instrument simulation (use at own risk!)

You can have ARCiS create simulated observations including estimate of the noise as function of wavelength.

> *Note that this is absolutely not intended as a replacement of a proper instrument simulation! It only includes photon noise and can be used to get a very rough estimate of the expected performance.*

instrument1:name Can be "MIRI", "NIRSPEC", "WFC3", "JWST" or "ARIEL". When it is something else it is assumed to be a filename containing a proper instrument simulation (file format currently the ExoSim format).

instrument1:ntrans Number of transits to average over. When put to 0, the number of transits is computed to assure that at each wavelength 7 scale-heights can be observed with 5σ accuracy.

5 Output files

There are many output files, most are for checking the model. The most important ones are discussed here.

log.dat This is the log file containing the runtime output.

input.dat Copy of the input file used appended with the command line keywords. This allows rerunning exactly this model again without command line keywords.

mixingratios.dat This file contains the temperature structure and the abundances of the molecules as a function of height in the atmosphere.

trans Transmission spectrum. Header explains units.

emis Emission spectrum. Header explains units.

emisR Emission spectrum relative to the stellar emission.

.txt File containing the MultiNest output when retrieval was done.

bestfit.dat File containing the input file for the best fitting model when retrieval was done.

6 Examples

There are a few examples in the Example directory downloaded with the git repository for retrieval and forward modelling.

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