Title

CEC

APPLICATION MANUAL

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SUMMARY

This document is the application manual of the CEC module. This module is dedicated to the computation of the droplets or particles flow field inside and outside the thruster. It is integrated in the PLUMFLOW procedure.

Chapter 3 presents the CEC module, chapter 4 describes in detail the input and output of the module, chapter 5 presents the CEC man-machine interface and chapter 6 gives an example of application.

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CEC V3.2 – Application Manual

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

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1 REFERENCE DOCUMENTS

[RD1] "Spécification d'intégration : PLUMFLOW, PLUME, CONTAMINE dans ESABASE". P. Chèoux-Damas, C. Theroude. Doc. MMS : S413/RT/17.94. 12/01/95.

[RD2] "PLUME V3.2 - Interface files definition". P. Chèoux-Damas. Doc. MMS : S413/RT/41.97. 24/10/97.

2 INTRODUCTION

The CEC module has two main objectives :

- To create of file containing the characteristics (mass, cross section, number of degrees of freedom) of groups of species for Monte-Carlo calculations (MCLIP, CONTAMINE, etc).
- To make a tool for managing the species groups available to the user.

The CEC module is integrated in the PLUMFLOW software and is interfaced with the ODE and MCLIP modules.

The CEC module is made on the one hand of a specific man-machine interface, on the other hand of a computation module for the generation of a file.

This document is the application manual of the CEC software. Chapter 2 presents the CEC module, chapter 3 describes in detail the input and output of the module, chapter 4 presents the CEC man-machine interface and chapter 5 gives an example of application.

3 CEC PRESENTATION

The CEC module is dedicated on the one hand to the management of groups of species, and on the other hand to the creation of a thermodynamic file containing the characteristics of the groups of species.

The development of the CEC module was performed to complete the capabilities of the existing ODE module that allows to evaluate the chemical equilibrium inside a thruster and to compute the thermodynamic properties of the gaseous mixture.

Indeed, the ODE outputs are not adapted to contamination calculations based on Monte-Carlo methods that require the properties of the species (cross section, number of degrees of freedom). Moreover, for contamination purpose, it could be interesting to modify the composition of the gaseous mixture in order to take into account specific species not computed by ODE (unburnt species, impurity).

The two following paragraphs present the two main functionalities of the CEC module.

3.1 MANAGEMENT OF THE CONTAMINANTS SPECIES

This function allows to create or modify a set of species groups for contamination analysis. The principles are the following :

- The list of the generated species is evaluated by the ODE software.
- The user can create using the CEC interface a set of species groups for contamination analysis. The minor species are suppressed. The species with similar properties (mass, etc) are gathered in the same group in order to limit the total number of groups.
- The user can add new species to the already existing list in order to take into account unburnt species, impurity, etc. He can also modify the molar fraction of each species in order to better model the real gaseous mixture.
- The CEC interface generates a namelist file allowing to run CEC and to compute the properties of each species group.

These operations can be performed using the CEC man-machine interface or by creating directly the namelist file.

3.2 GENERATION OF THE THERMODYNAMIC PROPERTIES

All the directives of computation are contained in the namelist file. The CEC execution allows to compute the thermodynamic properties of each species group. The principles of computation are the following :

- The viscosity of each species is evaluated from the VISCODE.DAT database and the mean viscosity of each group is then computed. The cross section and the exponent of variation are computed from the mean viscosity.
- The specific heat ratio (γ) of each species is evaluated from the JANNAF.THE database and the mean γ of each group is then computed. The number of degrees of freedom is computed from the mean γ.

The already existing databases JANNAF.THE and VISCODE.DAT can be completed by the user's data using two complementary databases (JANNAF.COMP and VISCODE.COMP).

4 CEC INPUT/OUTPUT

4.1 CEC ARCHITECTURE

The input files of the CEC software are the following :

- The run parameters file (.CEI). This file can be created either by the user or generated using the CEC man-machine interface.
- The thermodynamic file (.T07) generated by ODE,
- The thermodynamic data file (JANNAF.THE) that shall be present in the same directory as the executable,
- The viscosity data file (VISCODE.DAT) that shall be present in the same directory as the executable,
- The complementary thermodynamic data file (JANNAF.COMP) that is optional and shall be installed in the same directory as the executable. This file can be created by the user in order to add the thermodynamic properties of additional species to JANNAF.THE.
- The complementary viscosity data file (VISCODE.COMP) that is optional and shall be installed in the same directory as the executable. This file can be created by the user in order to add the viscosity properties of additional species to VISCODE.DAT.

These files are presented at the Figure 4.1-1 and detailed in the paragraph 4.2.

All these files are formatted in ASCII to allow the portability on different operating systems (HP, SUN, ULTRIX, etc).

The output files of the CEC software are :

- The listing file (.CEO) resuming the run parameters and the progress of the run,
- The thermodynamic file (.T07) generated by CEC,

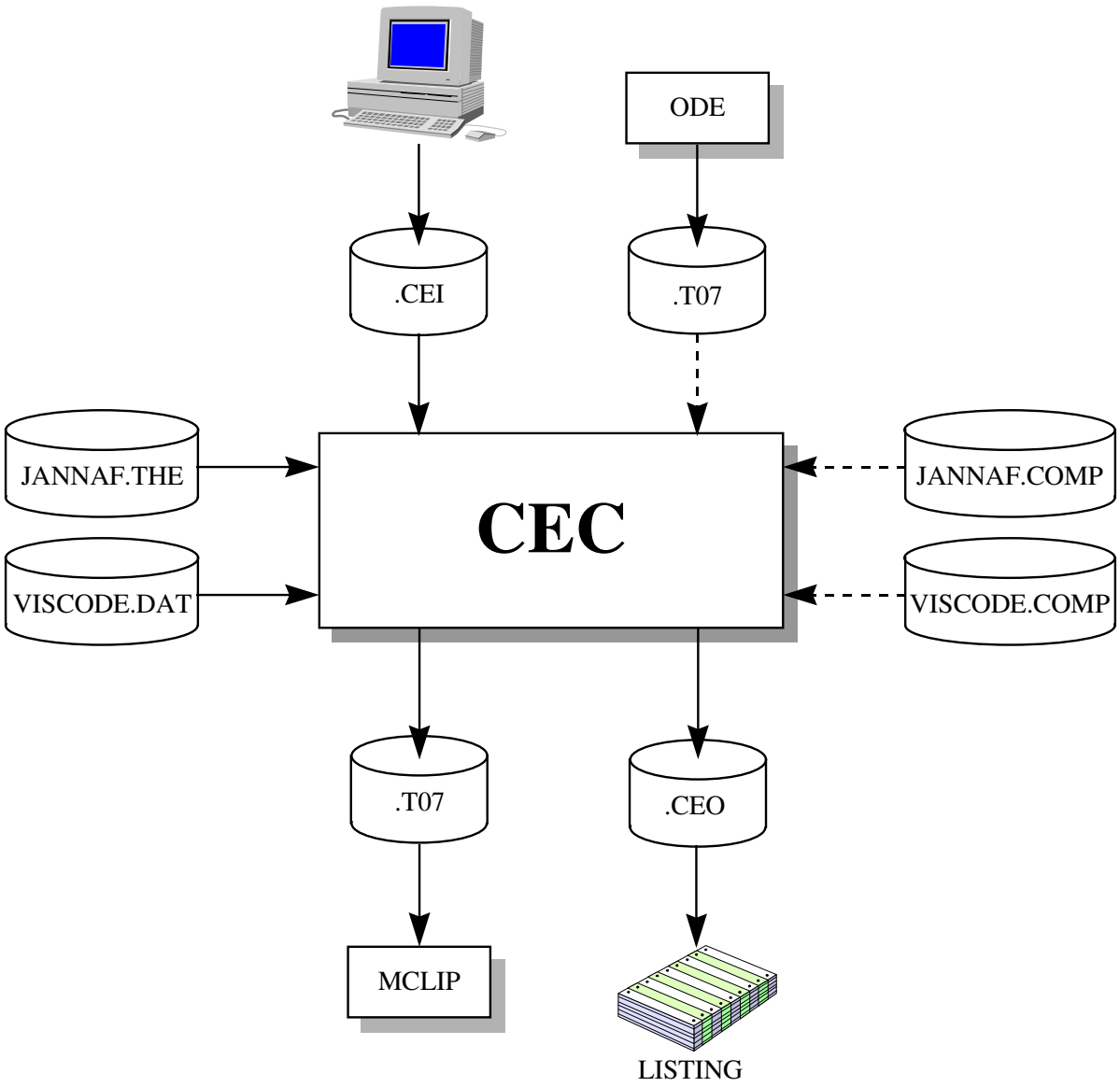


Figure 4.1-1 : Architecture of the CEC module

4.2 CEC INPUT FILES DESCRIPTION

4.2.1 The run parameters file : .CEI

This file contains the run parameters of the CEC software. It is characterised by its extension (.CEI). The structure of the run parameters file is based on a set of namelist.

The namelist, called $CEC is used to define the computation parameters.

The contents of the file is described hereafter.

Format of the file :

```
$CEC
TREF
NBGR
NAMEGR(I)          (I = 1,NBGR)
NBSP(I)            (I = 1,NBGR)
NAMESP(I,J)        (I = 1,NBGR), (J = 1, NBSP(I))
FMOLSP(I,J)        (I = 1,NBGR), (J = 1, NBSP(I))
$END
```

Description

$CEC part

TREF : Reference temperature for the computation of thermodynamic parameters (gamma, viscosity, etc).

Type : real

Unit : K

Default : 300.

NBGR : Number of group of species.

Type : integer

Range : ≤ 50

Default : 0

NAMEGR(I) : Name of the I^{th} group of species.

Type : character*12

NBSP(I) : Number of species of the Ith group.

Type : integer

Range : ≤ 50

Default : 0

NAMESP(J,I) : Name of the Jth species of the Ith group.

Type : character*12

FMOLSP(J,I) : Molar fraction of the Jth species of the Ith group.

Type : real

Range : ≤ 1.

Default : 0.

4.2.2 The thermodynamic file : .T07

This file contains the thermodynamic characteristics (mass, proportion, cross section, number of degrees of freedom) of each group of species. The complete description of the .T07 file is presented in the RD2.

This file is not mandatory but can be used as complement of the .CEI file.

4.2.3 The thermodynamic file : JANNAF.THE

This file is a table including the thermodynamic properties of about 700 chemical species. It is also used by ODE to compute the chemical equilibrium and the thermodynamic properties. This file shall be installed in the directory of the executable and shall not be modified by the user.

4.2.4 The viscosity file : VISCODE.DAT

This file is a table including the viscosity of about 200 chemical species. This file shall be installed in the directory of the executable and shall not be modified by the user.

4.2.5 The thermodynamic complementary file : JANNAF.COMP

This file allows the user to complete the JANNAF.THE file. It contains the specific heat of the species. The contents of the file is given hereafter.

Format of the file :

```
Comments line
Comments line
Comments line
Comments line
NAMESP
MOLAR_MASS       REF_TEMP          CPREF       EXPO
```

Description :

NAMESP : Name of the species.

Type : character*12

MOLAR_MASS : Molar mass of the species.

Type : real

Unit : g

REF_TEMP : Reference temperature.

Type : real

Unit : K

CPREF : Specific heat at constant pressure at the reference temperature.

Type : real

Unit : J/kg/K

EXPO : Exponent of the variation law of Cp.

Type : real

Unit : -

Remark :

The law of variation of the Cp is the following :

$$C_p(T) = CPREF.\left(\frac{T}{TREF}\right)^{EXPO}$$

4.2.6 The viscosity complementary file : VISCODE.COMP

This file allows the user to complete the VISCODE.DAT file. It contains the viscosity of the species. The contents of the file is given hereafter.

Format of the file :

```
Comments
Comments
Comments
Comments
NAMESP
REF_TEMP          VISCOREF          EXPO
```

Description :

NAMESP : Name of the species.

Type : character*12

REF_TEMP : Reference temperature.

Type : real

Unit : K

VISCOREF : Viscosity at the reference temperature.

Type : real

Unit : N.s/m^2

EXPO : Exponent of the variation law of the viscosity.

Type : real

Unit : -

Remark :

The law of variation of the viscosity is the Sutherland law :

$$\mu(T) = VISCOREF.\left(\frac{T}{TREF}\right)^{EXPO}$$

4.3 THE CEC OUTPUT FILES

4.3.1 The listing file : .CEO

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

An example of such a file is given hereafter. It contains :

- The description of the run parameters,
- The description of the databases used to perform the calculations,
- A summary of the .T07 file.

```
RUN DATA :
          COMMAND FILE  :                mbb10_new.CEI
          SPECIES FILE  :                mbb10_new.T07
     Computation of the species properties
     Group name : H2
     Species H2          was found in JANNAF.
     Species H2          was found in VISCODE.DAT.

     Group name : H2O
     Species H2O         was found in JANNAF.
     Species H2O         was found in VISCODE.DAT.

     Group name : N2+CO+C02
     Species CO          was found in JANNAF.
     Species CO          was found in VISCODE.DAT.
     Species CO2         was found in JANNAF.
     Species CO2         was found in VISCODE.DAT.
     Species N2          was found in JANNAF.
     Species N2          was found in VISCODE.DAT.

     .T07 FILE DESCRIPTION :
     ======================
     Reference temperature :  300.0000000 K

     Number of groups :   3

     Group name : H2
     Composition :      Species    Molar fraction
                         H2          .1950528E+00

     Group characteristics :
     Molar mass  Viscosity   Diameter   Exponent    Nb of DOF   Molar frac.
    .201594E+01 .886896E-05 .281947E-09 .186821E+00 .194379E+01 .195053E+00

     Group name : H2O
     Composition :      Species    Molar fraction
                         H2O         .4020337E+00

     Group characteristics :
     Molar mass  Viscosity   Diameter   Exponent    Nb of DOF   Molar frac.
    .180153E+02 .109411E-04 .478290E-09 .399474E+00 .307560E+01 .402034E+00

     Group name : N2+CO+C02
     Composition :      Species    Molar fraction
                         CO          .1621034E+00
                         CO2         .4575718E-01
                         N2          .1950528E+00

     Group characteristics :
      Molar mass  Viscosity   Diameter   Exponent    Nb of DOF   Molar frac.
    .298289E+02 .173241E-04 .406076E-09 .257032E+00 .222834E+01 .402913E+00
```

Extract of the .CEO file

4.3.2 The thermodynamic file : .T07

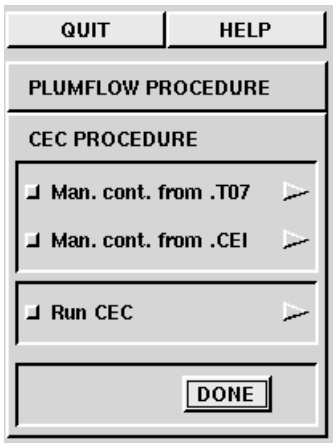
This file contains the thermodynamic characteristics (mass, proportion, cross section, number of degrees of freedom) of each group of species. The complete description of the .T07 file is presented in the RD2.

5 CEC MAN-MACHINE INTERFACE

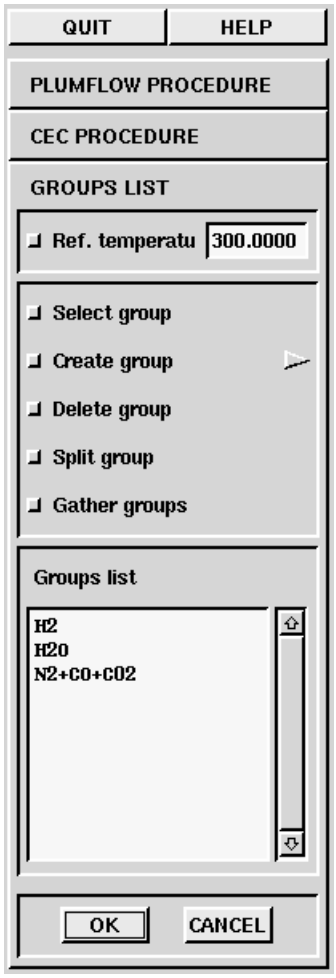
This paragraph presents the man-machine interface of the CEC module. The user access to the CEC menus by clicking on the ***CEC*** button in the main PLUMFLOW menu.

The CEC menus allow the user to create, modify and delete the groups of species.

The opposite menu is the main menu of the CEC module.



- The "manage contaminants from .T07" (***Man. cont. from .T07***) item allows the user to modify an already existing .T07 file. This option is available only if a .T07 file exists in the current directory.
- The "manage contaminants from .CEI" (***Man. cont. from .CEI***) item allows the user to create or modify an already existing .CEI file.
- The "***Run CEC"*** item allows to execute the CEC module in order to create a new .T07 file.

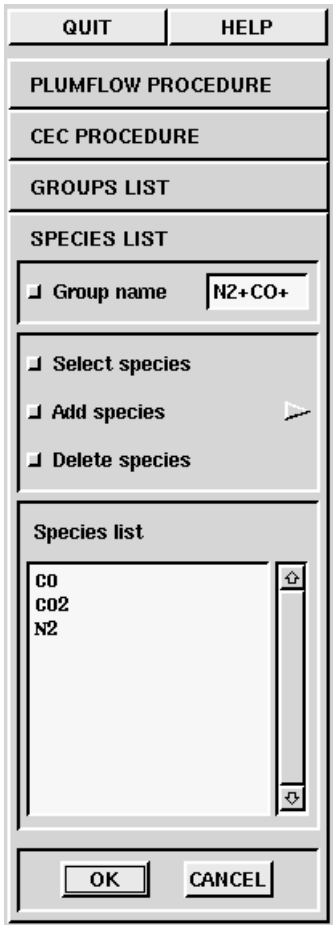


The opposite menu (***GROUPS LIST***) is dedicated to the modifications of the group of species.

- The "reference temperature" (***Ref. temperatu***) field allows to enter the temperature (in K) where the thermodynamic properties will be computed by the CEC application.
- The five next items allow to select, create, delete, split and gather groups.
- The bottom part of the menu is the list of the existing groups.
- To select a group, the user has to click in the list on the group he wants to select and then on ***Select group***.
- To create a group, the user has to click on ***Create group***.
- To delete groups, the user has to select the groups he wants to delete and then to click on ***Delete group***.
- To split a group, the user has to select the group he wants to split and then to click on ***Split group***. The CEC interface creates as much new groups as existing species in the selected group. By default, each new group has the name of the corresponding species.
- To gather groups, the user has to select the groups he wants to gather and then to click on ***Gather groups***. The CEC interface replaces the selected groups by a new group. By default, the new group name is the same as the first selected group.
- To validate the actions the user has to click on ***OK***.
- To go back to the preceding menus the user has to click on ***CANCEL***.

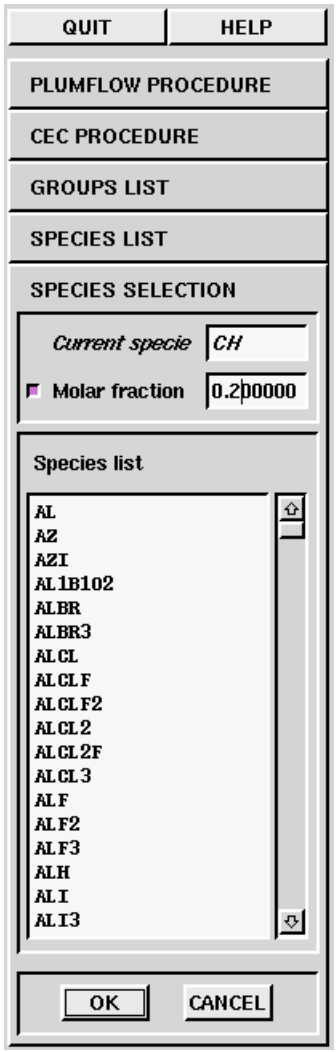
The opposite menu (***SPECIES LIST***) is dedicated to the modifications of the species included in a selected group.

- The ***Group name*** field can be modified by the user to modify the name of the selected group.
- The three next items allow to select, add and delete species.
- The bottom part of the menu is the list of species in the selected group.
- To select a species, the user has to click in the list on the species he wants to select and then on ***Select species***.
- To create a species, the user has to click on ***Add species***.
- To delete species, the user has to select the species he wants to delete and then to click on ***Delete species***.
- To validate the actions the user has to click on ***OK***.
- To go back to the preceding menus the user has to click on ***CANCEL***.



The opposite menu (***SPECIES SELECTION***) is dedicated to the modification of the species characteristics.

- The ***Current species*** field is the name of the species. This field cannot be directly entered by the user.
- The ***Molar fraction*** field is the molar fraction of the selected species. This field can be modified by the user.
- The ***species list*** is the list of the available species in the JANNAF database. To modify or to select a new species, the user has to select the species in the list and then to click on ***OK***. The ***Current species*** field is then updated.
- To validate the actions the user has to click on ***OK***.
- To go back to the preceding menus the user has to click on ***CANCEL***.



6 HOW TO USE CEC

The goal of this chapter is to present the use of the CEC module on a real case.

6.1 APPLICATION CASE

In this paragraph, a complete case of CEC application is presented. The goal of this case is to generate a .T07 file for MCLIP calculation.

6.1.1 External files

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

- A mbb10.T07 file computed by ODE.

6.1.2 Generation of the .CEI file

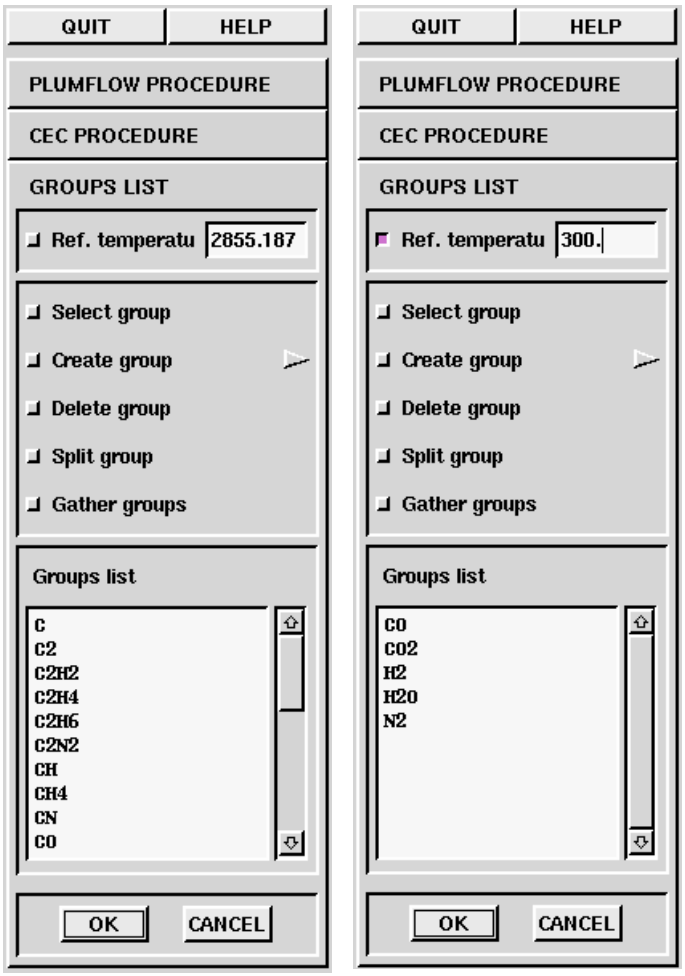
This paragraph describes how to generate a .CEI file using the CEC man-machine interface. In order to do that the user has to enter in the CEC menus by selecting ***CEC run*** in the PLUMFLOW main menu and then by selecting ***Man. cont. from .T07*** in the CEC main menu.

In the groups list menu, all the species created by ODE are displayed. First of all, the user has to delete all the minor species in order to keep the major species.

For the test case, the major species are H_2, H_2O, CO, CO_2 and N_2. So, the user has to select all the others species (C, C_2, C_2H_2, C_2H_4, C_2H_6, CH, CH_4, CN, H, HCN, H_2O_2, N, NH, NH_3, NO, N_2, N_2O, O, OH, O_2) and to click on ***Delete group.***

The reference temperature from ODE is the chamber temperature. This temperature does not correspond to the temperature of the external flow. So, the user has to modify the reference temperature by typing 300. In the ***Ref. temperatu*** field.

The two opposite figures are the menus before and after deleting the minor species.



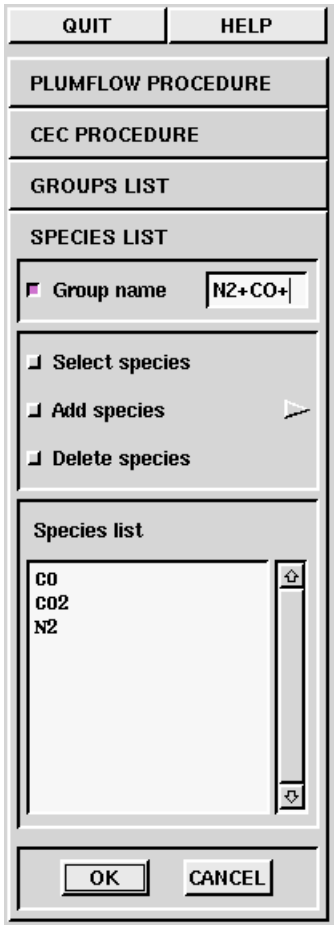
The second step is to gather some groups in order to reduce the number of groups for the future calculations. For the test case, three groups will be created : the light species group containing H_2, the mid-heavy species group containing H_2O and the heavy species group containing CO, CO_2 and N_2.

To do that, the user has to select the CO, CO_2 and N_2 groups in the groups list and click on ***Gather groups***. Then, only three groups remain in the list : CO, H_2 and H_2O.

The CO group contains the three heavy species and the user has to modify its name. To do that, the user has to select CO in the list and click on ***Select group***. He access to the species list menu and he can modify the group name by typing N2+CO+CO2 in the ***group name*** field and clicking on ***OK***.

The opposite figure gives the menu during the modification of the group name.

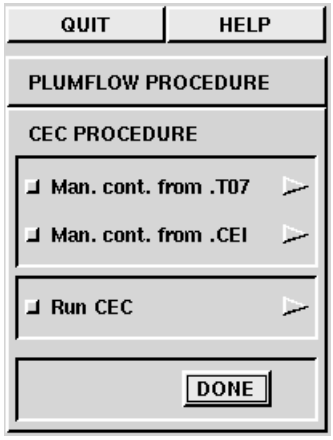
Then, the user has to go back to the main menu of CEC. Before quitting, the ***GROUPS LIST*** menu, the program asks the user a confirmation for the saving of the modifications in the .CEI file. The user has to answer ***YES*** to create the corresponding .CEI file.



6.1.3 Generation of the .T07 file

In the main CEC menu, the user has to click on ***Run CEC*** to create the .T07 file corresponding to the .CEI file created.

The opposite figure gives the main menu of CEC.



After achievement of the CEC execution the user can quit the CEC main menu and edit the .CEO file by typing ***Edit output files*** and then ***CEC***.

The .T07 file created by CEC is given hereafter.

```
300.0000        300.0000
   20.94655       1.4881912E-05  0.7953074       4.0718395E-10  0.2953074
   2.434911
H2
           1
H2
  0.1649028
   2.015940       8.8689612E-06  0.6868208       2.8194658E-10  0.1868208
   1.943795       0.1649028
H2O
           1
H2O
  0.3398872
   18.01534       1.0941092E-05  0.8994736       4.7828952E-10  0.3994736
   3.075598       0.3398872
N2+CO+CO2
           3
CO           CO2          N2
  0.1370444       3.8683869E-02  0.3194818
   29.26220       1.7430522E-05  0.7433988       4.0080028E-10  0.2433988
   2.158711       0.4952101
```

APPENDIX A - THEORETICAL ASPECTS

The theoretical aspects related to the computation of the macroscopic characteristics of the mixing are not presented here. The user can refer to the ODE application manual for more details.

The computation of the properties of the species groups is presented hereafter.

The knowledge of the macroscopic properties (viscosity, γ, etc) allows to perform computation in continuum medium (Navier-Stokes simulation, method of characteristics). On the other hand, the Monte-Carlo methods based on the simulation of the individual behaviour of molecules require the knowledge of the microscopic properties of the simulated species.

Thus, one of the functionalities of the CEC module is to compute the microscopic properties of the species from the macroscopic properties.

The formulae allowing the computation of the microscopic properties are the following :

- Evaluation of the cross section at the reference temperature :

$$\sigma_{ref} = \frac{15}{8} \frac{\left(\pi m k T_{ref}\right)^{1/2}}{\left(\Gamma(4-\alpha)\right)(2-\alpha)^{\omega} \mu_{ref}}$$

Where, T_{ref} is the reference temperature, μ_{ref} is the viscosity at the reference temperature, ω is the exponent of the Sutherland law and $\alpha = \omega - 0.5$.

Γ is the gamma function and is equal to :

$$\Gamma(j) = \int_0^{\infty} x^{j-1}.e^{-x}.dx$$

- Evaluation of the species diameter at the reference temperature :

$$d_{ref} = \sqrt{\frac{\sigma_{ref}}{\pi}}$$

- Evaluation of the exponent of the cross section law :

$$\alpha = \omega - 0.5$$

- Evaluation of the number of degrees of freedom :

$$n_{dof} = \frac{5-3\gamma}{\gamma-1}$$

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