Noncondensible Gas (NCG) Package
Users' Guide

Noncondensible gases (NCGs) in the Control Volume Hydrodynamics (CVH) package are modeled as ideal gases. The constant volume heat capacity is approximated as an analytic function of temperature. This document describes user input requirements for specifying a noncondensible gas to be present in calculation and defining or changing its equation of state.

More detailed information on the constitutive relations and the default values for the existing library of predefined noncondensible gases can be found in the NCG Reference Manual.

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1. Introduction

Noncondensible gases in the Control Volume Hydrodynamics (CVH) package are modeled as ideal gases and are characterized by their molecular weight, energy of formation, and specific heat capacity at constant volume, c_v, calculated from the general analytic form

$$c_v(T) = c_{v0} + c_{v1}T + c_{v2}T^2 + c_{v3}T^3 + \frac{c_{vsqrt}}{\sqrt{T}} + \frac{c_{vm1}}{T} + \frac{c_{vm2}}{T^2} \qquad (1.1)$$

for the temperature range $T_{low} \le T \le T_{up}$, and held fixed at the boundary value for temperatures below T_{low} or above T_{up}. Each of the coefficients in Equation (1.1), as well as T_{low} and T_{up}, can be specified via user input.

All MELCOR calculations are assumed to involve water in the pool, liquid water in the atmosphere and water vapor in the atmosphere. Because of this, water in the pool (which may be two-phase) is automatically defined as material number one, referred to as "POOL", liquid water in the atmosphere is automatically defined as material number two, referred to as "FOG", and water vapor in the atmosphere is automatically defined as material number three, referred to as "H2O-VAP". Noncondensible gases must be defined by the user as higher numbered materials if desired for a calculation. A library of data for gases of interest is available for use. The available gases and their associated coefficients for Equation (1.1) are defined in the NCG Reference Manual, and include hydrogen (H2), oxygen (O2), carbon dioxide (CO2), carbon monoxide (CO), nitrogen (N2), methane (CH4), helium (HE), argon (AR), and deuterium (D2).

Only the thermal equation of state of noncondensible gases is defined by the NCG package. The thermal equation of state for water is defined by the H2O package and is based on the analytic expression for the Helmholtz function, $\psi(\rho, T)$, that was used to generate the Keenan and Keyes Steam Tables. Transport properties such as viscosity, thermal conductivity, and binary diffusivity are treated in the Material Properties (MP) package. In order to evaluate the viscosity and thermal conductivity of control volume atmospheres, those properties must be defined for all noncondensible gases present in the calculation. Input to the MP package is therefore required in any calculation involving user-defined gases (GASA through GASJ). In addition, the user has the option of modifying the properties used for gases in the NCG default library.

2. MELGEN User Input

The user must specify which noncondensible gases are in the calculation and any desired changes in the default coefficients and other constants defining the equation of state (called "material properties" below). Liquid and vapor water are always materials one, two

and three and do not need to be defined for a calculation. To include a material in the calculation, a record of the following form must be in the MELGEN input:

NCGnnn – Identifier Field
000 ≤ nnn ≤ zzz used for ordering
Required

The minimum amount of information is the MELCOR name and material number. Library data are used unless the user inputs the material property data. Material property data is input pairwise. The first data pair identifies the material property and the second is the material property value. An arbitrary number of data pairs may be input on a single record but a data pair may not be split across two records. More than one record may have the same MELCOR name and material number if more than one are required to define the material properties. Although they need not be defined in order, no gaps in the material numbers are allowed. Water and steam are always materials one through three. All data for user-defined gases GASA-GASJ must be input.

(1) MNAME - MELCOR material name, e.g., O2 for oxygen.
(type = character, default = none, units = dimensionless)

(2) MNUMBER - MELCOR material number. This material will be referred to by this number through the calculation.
(type = integer, default = none, units = dimensionless)

(3) MP NAME - Material property name. Refer to the following table of allowed material properties.
(type = character, default = none, units = dimensionless)

(4) MP VALUE - Material property value. Refer to the following table for units.
(type = real, default = none, units = depends on property)

.
.
.
additional MP NAME/VALUE pairs

Material Property Name	Units	Physical Interpretation
CV0	J/(kg K)	c_{v0} coefficient in $c_v(T)$
CV1	J/(kg K^2)	c_{v1} coefficient in $c_v(T)$
CV2	J/(kg K^3)	c_{v2} coefficient in $c_v(T)$
CV3	J/(kg K^4)	c_{v3} coefficient in $c_v(T)$

Material Property Name	Units	Physical Interpretation
CVSQRT	$J/(kg\sqrt{K})$	c_{vsqrt} coefficient in $c_v(T)$
CVM1	J/kg	c_{vm1} coefficient in $c_v(T)$
CVM2	(J K)/kg	c_{vm2} coefficient in $c_v(T)$
TLOW	K	T_{low} lowest temperature for fit to $c_v(T)$
TUP	K	T_{up} highest temperature for fit to $c_v(T)$
WM	kg/mol	molecular weight
EF	J/kg	e_f energy of formation
SZ	J/(kg K)	s_0 entropy at natural temperature (not used currently)

After all the records have been processed, all material numbers between 1 and the largest number used as a hydrodynamic material number in CVH input must be defined. (Of course, materials 1, 2, and 3 are automatically defined.) There can be no gaps in the material numbers. For example, if only materials one, two, three and six are defined, then an error will occur because materials four and five are not defined.

3. MELCOR User Input

Currently, the noncondensible gases database and models cannot be changed via MELCOR input.

4. Sensitivity Coefficients

The *sensitivity coefficient* feature in MELCOR is a powerful feature that gives the user the ability to change selected parameters the physics models that would otherwise require modification of the Fortran source code. Their use is described in Section 7 of the MELCOR EXEC Users' Guide.

4.1 NCG Sensitivity Coefficients

Only one sensitivity coefficient is used. It is the temperature T_n that appears in the integral of specific heat $c_v(T)$ to determine the specific internal energy and enthalpy (see the NCG Reference Manual).

2090 – Natural Temperature

(1) - The lower temperature limit used in the integral of $c_v(T)$ to calculate specific internal energy and enthalpy.

(default = 298.15, units = K, equiv = none)

5. Plot Variables and Control Function Arguments

There are no plot variables or control function arguments for the NCG package.

6. Example Input

Materials one, two, and three are always water in the pool (may be two-phase), liquid water in the atmosphere (fog), and water vapor in the atmosphere, respectively. The example input set below defines four as hydrogen and material five as oxygen with a modified value for c_{v0} of 3000. Note that the sequencing order does not matter as long as there are no gaps in material numbers after completion of NCG processing.

```
NCG000    O2   5    CV0  3000.
NCG010    H2   4
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7. Example Output

No example output is included in this document.

8. Diagnostic and Error Messages

Diagnostic and error messages can originate from bad user input. The messages will be self-explanatory.