

Noncondensable Gas (NCG) and Water (H2O) Packages Reference Manual

Noncondensable gases 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. The equation of state for water is based on the analytic expression for the Helmholtz function used to generate the familiar Keenan and Keyes Steam Tables. [1] This document describes the constitutive relations used for the water and noncondensable gases equations of state, and it lists the default values of the associated constants for the gases provided in the NCG library.

User input requirements for the NCG package are described in the NCG Users' Guide. There is no input allowed for the H2O package.

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1. NCG Equation of State

Noncondensable gases in the Control Volume Hydrodynamics (CVH) package are modeled as ideal gases. The specific internal energy and enthalpy of an ideal gas is a function only of its temperature, T , the natural state (reference) temperature, T_n , its energy of formation, e_{form} , its enthalpy of formation, h_{form} , the universal gas constant, R , and its molecular weight, w .

$$e(T) = \int_{T_n}^T c_v(T') dT' + e_{form} \quad (1.1)$$

$$h(T) = \int_{T_n}^T \left(c_v(T') + \frac{R}{W} \right) dT' + h_{form} \quad (1.2)$$

The pressure, P , is a function of the mass density, ρ , the temperature, T , the universal gas constant, R , and the molecular weight, w ,

$$P = \frac{\rho R T}{w} \quad (1.3)$$

The noncondensable gases in MELCOR are characterized by the temperature dependent constant volume specific heat, $c_v(T)$, the natural state (reference) temperature, T_n , the energy of formation, e_{form} , the entropy at the reference temperature, s_0 (this quantity is not currently used in the calculation but is included for completeness), and the molecular weight of the material, w .

The specific heat for each noncondensable gas calculated from an analytic fit in the general form

$$c_v(T) = c_{v0} + c_{v1}T + c_{v2}T^2 + c_{v3}T^3 + \frac{c_{vsqrt}}{\sqrt{T}} + \frac{c_{vm1}}{T} + \frac{c_{vm2}}{T^2} \quad (1.4)$$

for the temperature range $T_{low} \leq T \leq T_{up}$, where T_{low} and T_{up} may be different for each gas. The value at T_{low} is used for $T < T_{low}$, and the value at T_{up} is used for $T > T_{up}$.

Using this constitutive relation for the specific heat, the internal energy is given by

$$e(T) = e_0 + c_{v0}T + \frac{1}{2}c_{v1}T^2 + \frac{1}{3}c_{v2}T^3 + \frac{1}{4}c_{v3}T^4 + 2c_{vsqrt}\sqrt{T} + c_{vm1}\ln(T) - \frac{c_{vm2}}{T} \quad (1.5)$$

for $T_{low} \leq T \leq T_{up}$, and is extrapolated outside that range using the constant limiting specific heat at T_{low} or T_{up} are used. Here

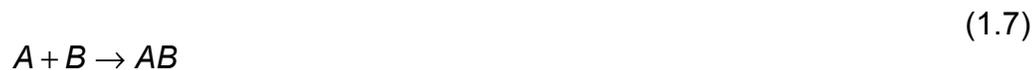
$$e_0 = e_{form} - c_{v0}T_n - \frac{1}{2}c_{v1}T_n^2 - \frac{1}{3}c_{v2}T_n^3 - \frac{1}{4}c_{v3}T_n^4 - 2c_{vsqrt}\sqrt{T_n} - c_{vm1}\ln(T_n) + \frac{c_{vm2}}{T_n} \quad (1.6)$$

Each of the coefficients can be specified via user input, as described in the NCG Users' Guide. Appropriate default coefficients for gases of interest from JANAF [2] and other sources are included in the noncondensable gas equation of state library, as described in Section 2. The default natural temperature used is 298.15 K; this may be changed with sensitivity coefficient 2090.

The reader may note that the definition of e_0 is actually inconsistent unless T_n lies in the range $T_{low} \leq T_n \leq T_{hi}$. For a number of gases (N_2 , O_2 , CH_4 , CO and CO_2), T_{low} is 300 K while T_n is 298.15. In these cases, the discrepancy is less than 10 J/kg and is totally insignificant compared to heats of reaction (several MJ/kg). Although the discrepancy for D_2 ($T_{low} = 600$ K) is significantly greater, this gas is not used in light water reactor simulations.

1.1 Integration Constants in the Energy Function

A modified thermochemical reference point is used in the NCG package. That is, all heats of formation of compounds are included in the enthalpy functions, as in JANAF tables. The advantage is that all heats of reaction are implicitly contained in the enthalpy functions. For example, in a reaction



taking place at constant temperature and pressure, total enthalpy is conserved. The heat released is the difference between the enthalpy of the reactants and that of the products. This is simply the chemists' definition of the heat of reaction,

$$Q_R(T) = h_A(P, T) + h_B(P, T) - h_{AB}(P, T) \quad (1.8)$$

Therefore, chemical reactions (such as gas combustion simulated by the Burn package) can be treated simply as changes in the masses of various materials; the associated heat effects are accounted for automatically through the equations of state.

Since only differences in enthalpy are significant, one integration constant may be chosen for each element represented in the collection of gases in the database. Conventional practice is to choose these integration constants such that the enthalpy of each element is zero in its standard state (25°C, 1 atm, with the material in its most stable state). However, water properties in MELCOR are defined (in the H2O package) consistent with Keenan and Keyes Steam Tables [1], as discussed in Section 2. Because water is formed from hydrogen and oxygen, the integration constants for hydrogen, oxygen, and water may *not* be chosen independently. The conventional integration constant is used for hydrogen in the NCG package, but the integration constant for oxygen has therefore been chosen such that the reference point for water vapor is consistent with that used by Keenan and Keyes. This results in a shift in the integration constant for every oxygen-containing gas in the NCG package compared to its conventional JANAF value. For all other gases, the integration constants are consistent with conventional practice.

In actuality, the reference point used will be significant only if a gas is chemically active. For current MELCOR models, the only such gases are H₂, D₂, O₂, CO, CO₂, and CH₄. (CH₄ is active *only* if the B₄C reaction in the COR package is enabled, in which case the heat of reaction data used there are not fully compatible with NCG data.) Thus, the user need not worry much about the reference points for other (in particular, user-defined) gases. If chemically active gases are modified, the reference point energy must not be arbitrarily redefined.

2. H2O Equation of State

The equation of state for water is based on the analytic expression for the Helmholtz function, $\psi(\rho, T)$, that was used to generate the familiar Keenan and Keyes Steam Tables [1]. The expression, involving a double power series with log and exponential terms, may be found in the Appendix to the 1969 tables. It contains approximately 50 constant coefficients. These cannot be changed in MELCOR.

The Keenan and Keyes formulation is augmented by JANAF data [2] for temperatures greater than 1589 K (2400 °F). The resulting equation of state is valid for temperatures greater than 273.15 K and for pressures less than 100 MPa.

2.1 Single-Phase Properties

The H2O package determines all single-phase thermodynamic properties of water as functions of density and temperature from the equation for ψ . For example, pressure and internal energy may be expressed in terms of the first derivatives of ψ as

$$P = \rho^2 (\partial \psi / \partial \rho)_T \quad (2.1)$$

$$e = \psi + T s = \psi - T (\partial \psi / \partial T)_\rho \quad (2.2)$$

where s is entropy. These are evaluated from the equation for ψ and those for its analytic term-by-term derivatives. The quantities $(\partial P / \partial T)_\rho$, $(\partial P / \partial \rho)_T$, and $c_v = (\partial e / \partial T)_\rho$, which involve the three independent second derivatives of ψ , are evaluated similarly.

2.2 Mixed-Phase Properties

The coexistence curve (the saturation line) is defined by points where P , T , and the Gibbs function $g = \psi + P / \rho$ are equal for two different values of ρ . This curve was determined by a calculation external to MELCOR. All properties of each phase were tabulated at 1 K intervals and are included as data in the H2O package. The properties of two-phase states are evaluated from these tables, using the lever rule.

3. NCG Library

A library of data for gases of interest is available for use. Any of the numbers may be changed via user input. The available gases and the associated constants are defined below. Ten user-defined gases called GASK, where k is any letter from A to J, can also be used, but the user must define all the values for the associated constants. Units for the parameters are given in the NCG Users Guide.

Hydrogen (H₂)	
	MELCOR Name: H2
	Molecular Weight: 0.0020162
C_{v0} :	-17849.
C_{v1} :	11.28298
C_{v2} :	-2.1081958E-3
C_{v3} :	1.5635602E-7
C_{vsqrt} :	865616.
C_{vm1} :	-8188058.3
C_{vm2} :	1.925734E8
T_{low} :	100.
T_{up} :	6000.
e_f :	0.
s_0 :	0.

Deuterium (D₂)	
	MELCOR Name: D2
	Molecular Weight: 0.00400
C_{v0} :	5508.8
C_{v1} :	-2.0277
C_{v2} :	3.3827E-3
C_{v3} :	-1.0842E-6
C_{vsqrt} :	0.
C_{vm1} :	0.
C_{vm2} :	0.
T_{low} :	600.
T_{up} :	1500.
e_f :	0.
s_0 :	0.

Helium (He)	
	MELCOR Name: HE
	Molecular Weight: 0.004003
C_{v0} :	5231.0
C_{v1} :	0.
C_{v2} :	0.
C_{v3} :	0.
C_{vsqrt} :	0.
C_{vm1} :	0.
C_{vm2} :	0.

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	T_{low} :	1.
	T_{up} :	10000.
	e_f :	0.
	s_0 :	0.

Nitrogen (N₂)		
	MELCOR Name: N2	
	Molecular Weight: 0.02801	
	C_{v0} :	1.117E3
	C_{v1} :	0.
	C_{v2} :	0.
	C_{v3} :	0.
	C_{vsqrt} :	0.
	C_{vm1} :	-2.880E5
	C_{vm2} :	5.348E7
	T_{low} :	300.
	T_{up} :	5000.
	e_f :	0.
	s_0 :	0.

Oxygen (O₂)		
	MELCOR Name: O2	
	Molecular Weight: 0.032	
	C_{v0} :	1245.
	C_{v1} :	0.
	C_{v2} :	0.
	C_{v3} :	0.
	C_{vsqrt} :	-16763.
	C_{vm1} :	1.111E5
	C_{vm2} :	0.
	T_{low} :	300.
	T_{up} :	2778.
	e_f :	1.7828E7
	s_0 :	0.

Argon (Ar)		
	MELCOR Name: AR	
	Molecular Weight: 0.03994	
	C_{v0} :	525.26
	C_{v1} :	0.
	C_{v2} :	0.
	C_{v3} :	0.
	C_{vsqrt} :	0.
	C_{vm1} :	0.
	C_{vm2} :	0.
	T_{low} :	1.
	T_{up} :	10000.
	e_f :	0.
	S_0 :	0.

Methane (CH₄)		
	MELCOR Name: CH4	
	Molecular Weight: 0.0160324	
	C_{v0} :	660.6
	C_{v1} :	3.462
	C_{v2} :	0.
	C_{v3} :	0.
	C_{vsqrt} :	0.
	C_{vm1} :	0.
	C_{vm2} :	0.
	T_{low} :	300.
	T_{up} :	833.
	e_f :	-4.5153E6
	S_0 :	0.

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Carbon Monoxide (CO)		
	MELCOR Name: CO	
	Molecular Weight: 0.028	
	c_{v0} :	1.116E3
	c_{v1} :	0.
	c_{v2} :	0.
	c_{v3} :	0.
	c_{vsqrt} :	0.
	c_{vm1} :	-2.7312E5
	c_{vm2} :	4.9348E7
	T_{low} :	300.
	T_{up} :	5000.
	e_f :	6.3286E6
	s_0 :	0.

Carbon Dioxide (CO₂)		
	MELCOR Name: CO2	
	Molecular Weight: 0.044	
	c_{v0} :	1351.35
	c_{v1} :	0.
	c_{v2} :	0.
	c_{v3} :	0.
	c_{vsqrt} :	0.
	c_{vm1} :	-3.4497E5
	c_{vm2} :	4.138E7
	T_{low} :	300.
	T_{up} :	3500.
	e_f :	4.0785E6
	s_0 :	0.

Acetylene (C₂H₂)		
	MELCOR Name: C2H2	
	Molecular Weight: 0.026016	
	<i>c_{v0}</i> :	1.1457E3
	<i>c_{v1}</i> :	0.
	<i>c_{v2}</i> :	0.
	<i>c_{v3}</i> :	0.
	<i>c_{vsqrt}</i> :	0.
	<i>c_{vm1}</i> :	0.
	<i>c_{vm2}</i> :	0.
	<i>T_{low}</i> :	1.
	<i>T_{up}</i> :	10000.
	<i>e_f</i> :	8.8104E6
	<i>s₀</i> :	0.

Ethylene (C₂H₄)		
	MELCOR Name: C2H4	
	Molecular Weight: 0.028032	
	<i>c_{v0}</i> :	334.51
	<i>c_{v1}</i> :	1.7568
	<i>c_{v2}</i> :	0.
	<i>c_{v3}</i> :	0.
	<i>c_{vsqrt}</i> :	0.
	<i>c_{vm1}</i> :	0.
	<i>c_{vm2}</i> :	0.
	<i>T_{low}</i> :	194.
	<i>T_{up}</i> :	611.1
	<i>e_f</i> :	1.9536E6
	<i>s₀</i> :	0.

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Ammonia (NH₃)		
	MELCOR Name: NH3	
	Molecular Weight: 0.017029	
	<i>c_{v0}</i> :	1.7012E3
	<i>c_{v1}</i> :	0.
	<i>c_{v2}</i> :	0.
	<i>c_{v3}</i> :	0.
	<i>c_{vsqrt}</i> :	0.
	<i>c_{vm1}</i> :	0.
	<i>c_{vm2}</i> :	0.
	<i>T_{low}</i> :	1.
	<i>T_{up}</i> :	10000.
	<i>e_f</i> :	-2.557E6
	<i>s₀</i> :	0.

Nitrogen Monoxide (NO)		
	MELCOR Name: NO	
	Molecular Weight: 0.03005	
	<i>c_{v0}</i> :	6.8985E2
	<i>c_{v1}</i> :	0.
	<i>c_{v2}</i> :	0.
	<i>c_{v3}</i> :	0.
	<i>c_{vsqrt}</i> :	0.
	<i>c_{vm1}</i> :	0.
	<i>c_{vm2}</i> :	0.
	<i>T_{low}</i> :	1.
	<i>T_{up}</i> :	10000.
	<i>e_f</i> :	6.561E6
	<i>s₀</i> :	0.

Nitrous Oxide (N₂O)		
	MELCOR Name: N2O	
	Molecular Weight: 0.04401	
	<i>C_{v0}</i> :	736.32
	<i>C_{v1}</i> :	0.
	<i>C_{v2}</i> :	0.
	<i>C_{v3}</i> :	0.
	<i>C_{vsqrt}</i> :	0.
	<i>C_{vm1}</i> :	0.
	<i>C_{vm2}</i> :	0.
	<i>T_{low}</i> :	1.
	<i>T_{up}</i> :	10000.
	<i>e_f</i> :	4.6699E6
	<i>S₀</i> :	0.

User Defined Gases (-)		
	MELCOR Name: GASK, k = A, B, ... , J	
	Molecular Weight: -1.	
	<i>C_{v0}</i> :	-1.
	<i>C_{v1}</i> :	-1.
	<i>C_{v2}</i> :	-1.
	<i>C_{v3}</i> :	-1.
	<i>C_{vsqrt}</i> :	-1.
	<i>C_{vm1}</i> :	-1.
	<i>C_{vm2}</i> :	-1.
	<i>T_{low}</i> :	-1.
	<i>T_{up}</i> :	-1.
	<i>e_f</i> :	-1.
	<i>S₀</i> :	-1.

References

1. J. H. Keenan, et al., Steam Tables: Thermodynamic Properties of Water, Including Vapor, Liquid, and Solid Phases (SI Units), John Wiley & Sons, Inc., New York (1978).
2. JANAF Thermochemical Tables, Dow Chemical Company, Thermal Research Laboratory, Midland, MI (1965).