Sandia National Laboratories

Securing the future of Nuclear Energy

MELCOR

MELCOR 2.X for Fusion – EOS, NCG, and CVH

2025 European MELCOR Users' Group Meeting

April 7th-11th, 2025

U.S.NRC

SAND2025-04009PE

Overview

Review “fluids” or hydrodynamic materials as they pertain to MELCOR for fusion

- Noncondensable gases (NCG)
  - Theoretical aspects
  - Built-ins and defaults
  - User capabilities
- Condensable working fluids (EOS)
  - Package mechanics
  - Built-ins and defaults
  - User capabilities
  - Liquid freezing

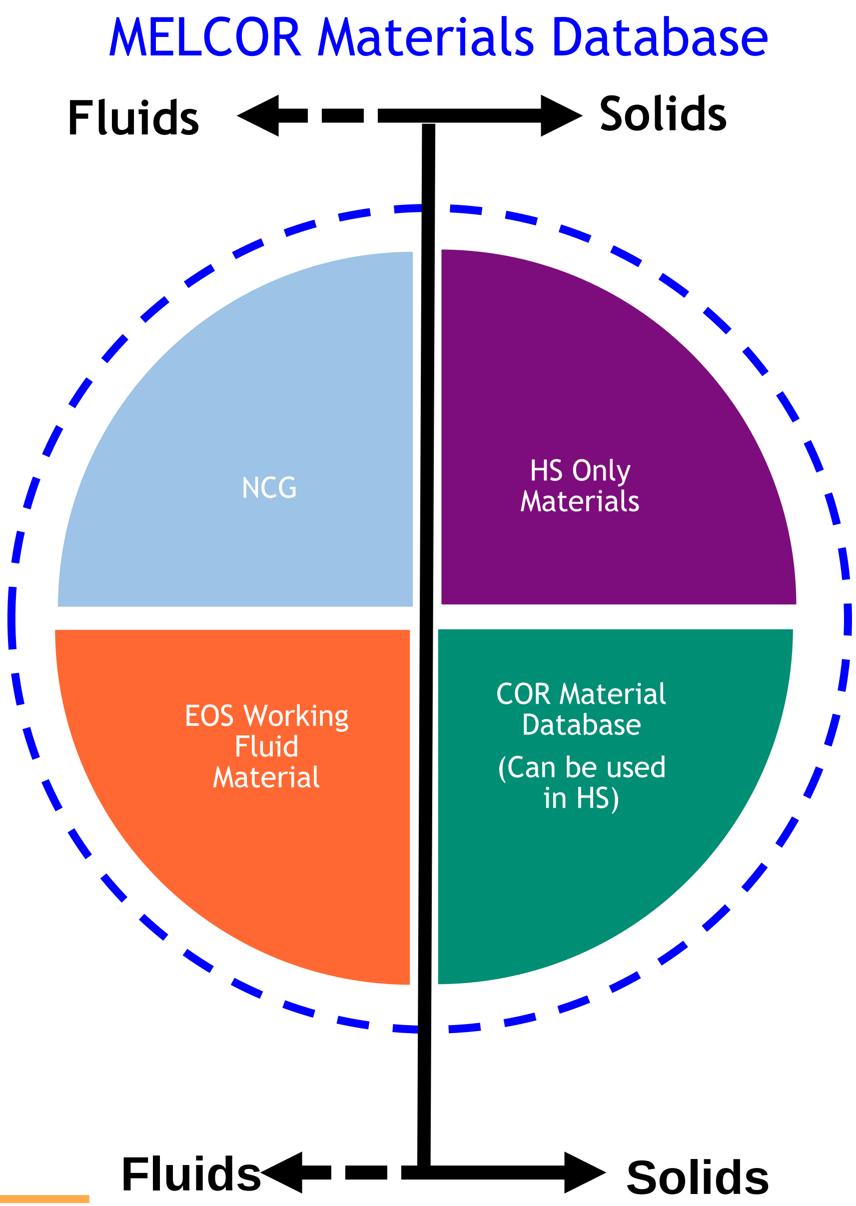
Compare NCG/EOS modeling between MELCOR 2.X and MELCOR (1.8.6) for fusion

Modeling/capabilities development for fluids in MELCOR 2.X for fusion

Summary

MELCOR Materials

AR
H2
HE
AR
D2
O2
CO2
CO
N2
NO
N2O
NH3
C2H2
CH4
C2H4
WATER
STEAM
NON-LWR



Zircaloy (ZR)
Zirconium Oxide (ZRO2)
Zirconium Oxide (ZRO2-INT)
Uranium Dioxide (UO2)
Uranium Dioxide (UO2-INT)
Stainless Steel (SS)
Stainless Steel Oxide (SSOX)
Boron Carbide (B4C)
Boron Carbide (B4C-INT)
Silver-Indium-Cadmium (AGINC)
Uranium Metal (UMETL)
Graphite (GRAPH)
Concrete (CON)
Aluminum (ALUM)
Aluminum Oxide (AL2O3)
Cadmium (CADM)
Stainless Steel 304 (SS304)
Lithium Aluminum (LIAL)
Uranium Aluminum (UAL)
Carbon Steel (CS)

NCG – Enthalpy and Internal Energy

MELCOR

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 $c_v(T)$
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

Enthalpy: $h\,(T) = \int_{T_n}^{T} \left(C_v(T') + \frac{R}{w} \right) dT' + h_{form}$

Internal Energy: $e(T) = \int_{T_n}^{T} C_v(T')dT' + e_{form}$

Fit to C_v: $C_v(T) = C_{v0} + C_{v1}T + C_{v2}T^2 + C_{v3}T^3 + \frac{C_{vsqrt}}{\sqrt{T}} + \frac{C_{vm1}}{T} + \frac{C_{vm2}}{T^2}$

Implementation:

- Internal energy integration

$$e(T) = e_0 + C_{v0}T + \frac{C_{v1}T^2}{2} + \frac{C_{v2}T^3}{3} + \frac{C_{v3}T^4}{4} + 2C_{vsqrt}\sqrt{T} + C_{vm1}\ln(T) + \frac{C_{vm2}}{T} + e_{form}$$

$T_{low} \le T \le T_{up}$; e(T) extrapolated outside that range using the constant limiting specific heat at T_{low} or T_{up}

- Energy of formation:

$$e_0 = e_{form} - \left(C_{v0}T_n + \frac{C_{v1}{T_n}^2}{2} + \frac{C_{v2}{T_n}^3}{3} + \frac{C_{v3}{T_n}^4}{4} + 2C_{vsqrt}\sqrt{T_n} + C_{vm1}\ln(T_n) - \frac{C_{vm2}}{T_n} \right)$$

- Chemical reactions and heats of reaction
  - Heats of formation of compounds are included in enthalpy functions
  - All heats of reaction implicitly contained in enthalpy functions
  - Chemical reactions treated as simple changes of mass with heat effects captured by EOS

$$A + B \Rightarrow AB$$
$$Q_R(T) = h_A(P,T) + h_B(P,T) - h_{AB}(P,T)$$

NCG – Dynamic Viscosity

Tabular Functions

- Default/built-in as functions of temperature for water, steam, air, hydrogen, deuterium
- User definitions – NCG_PRP to specify rule (CF or TF) or switch rule (Chapman-Enskog)

Chapman-Enskog for low-pressure pure gas

$$\mu_i = \left(2.6693 * 10^{-6}\right)\left(\frac{\sqrt{1000MT}}{\sigma^2 \Omega_v}\right)$$

- Lennard-Jones potential parameter dependence
  - Collision diameter – defaults for each default NCG
  - ε/k - defaults for each default NCG
  - User can redefine either/or
  - Collision integral table look-up for $0.3 \le T^* < 100$

Chapman-Enskog for mix of low-pressure gases

$$\mu_{mix} = \sum_{i=1}^{n}\left(\frac{y_i \mu_i}{\sum_{j=1}^{n} y_j \varphi_{ij}}\right)$$

Where:

M	=	Molecular weight [kg/mol]
T	=	Gas Temperature [K]
σ	=	Collision diameter [10^{-10} m]
Ω_v	=	Collision integral
	=	$\begin{cases} 2.785\left(\frac{T^*}{0.3}\right)^{-0.4}, & T^* < 0.3 \\ f(T^*), & 0.3 \le T^* < 100 \\ 0.5882\left(\frac{T^*}{100}\right)^{-0.145}, & T^* \ge 100 \end{cases}$
T^*	=	$\frac{kT}{\varepsilon}$
$\frac{\varepsilon}{k}$	=	Characteristic energy / Boltzmann's constant [K]
y_i	=	Mole fraction of gas i
M_i	=	Molecular weight of gas i
φ_{ij}	=	$\left(\frac{1}{\sqrt{8}}\right)\left(\frac{M_j}{M_i}\right)\left(\frac{M_i}{M_j+M_i}\right)^{1/2}\left[\left(\frac{M_i}{M_j}\right)^{1/4}+\left(\frac{\mu_i}{\mu_j}\right)^{1/2}\right]^2$

Equation fit

- Power laws for air, helium, nitrogen, oxygen, and argon: $\mu_i = A_i T^{B_i}$
- "Dilute region" where ideal gas law applicable
- Wilke method for gas mixtures (similar formulation to Chapman-Enskog for mixtures)

NCG – Thermal Conductivity

Tabular Functions

- Default/built-in as functions of temperature for water, steam, air
- User definitions – NCG_PRP to specify rule (CF or TF) or switch rule

Eucken correlation for pure gas using Chapman-Enskog dynamic viscosity

$$\lambda_i = \left(C_{vi} + \frac{9R}{4M_i} \right) \mu_i$$

Wassijewa equation for mix of low-pressure gases

$$\lambda_{mix} = \sum_{i=1}^{n} \left(\frac{y_i \lambda_i}{\sum_{j=1}^{n} y_j A_{ij}} \right)$$

Where:

C_{vi}	=	Heat capacity at constant volume [J/kg/K]
R	=	Universal gas constant = 8.31441 [J/mol/K]
μ_i	=	Dynamic viscosity [kg/m/s]
M_i	=	Molecular weight of gas i [kg/mol]
y_i	=	Mole fraction of gas i
A_{ij}	=	$\left(\frac{1}{\sqrt{8}}\right)\left(\frac{M_j}{M_i}\right)\left(\frac{M_i}{M_j+M_i}\right)^{1/2}\left[\left(\frac{M_i}{M_j}\right)^{1/4}+\left(\frac{\mu_i}{\mu_j}\right)^{1/2}\right]^2$

Equation fit

- Power laws for air, helium, nitrogen, oxygen, and argon: $\lambda_i = A_i T^{B_i}$
- “Dilute region” where ideal gas law applicable
- Wassijewa method for gas mixtures
- Helium also has a fit from KTA rules:

$$\lambda_{He} = \left(2.682 * 10^{-3}\right)\left(1 + 1.123 * 10^{-8} P\right)\left(T^{0.71}\right)\left(1 - 2 * 10^{-9} P\right)$$

NCG – Binary Diffusion Coefficient

CVH, HS, and COR utilize correlations for steam/air and steam/hydrogen

- Steam/air:

$$D = (4.7931 * 10^{-5})\left(\frac{T^{1.9}}{P}\right)$$

- Steam/hydrogen:

$$D = (6.60639 * 10^{-4})\left(\frac{T^{1.68}}{P}\right)$$

Chapman-Enskog, low-pressure gases

$$D_{ij} = (1{,}88292 * 10^{-2})\left(\frac{\sqrt{T^3\left(\frac{0.001}{M_i} + \frac{0.001}{M_j}\right)}}{P\sigma_{ij}^2\Omega_{D,ij}}\right)$$

Where:

$M_{i\|j}$	=	Molecular weight of gas $i\|j$ [kg/mol]
T	=	Gas Temperature [K]
P	=	Gas Pressure [Pa]
$\sigma_{i\|j}$	=	Collision diameter of gas $i\|j$ [10^{-10} m]
σ_{ij}	=	Effective collision diameter of gas i and j [10^{-10} m]
	=	$\frac{1}{2}(\sigma_i + \sigma_j)$
$\Omega_{D,ij}$	=	Collision integral
	=	$\begin{cases} 2.662\left(\frac{T_{ij}^*}{0.3}\right)^{-0.5}, & T_{ij}^* < 0.3 \\ f(T_{ij}^*), & 0.3 \le T_{ij}^* < 100 \\ 0.5170\left(\frac{T_{ij}^*}{100}\right)^{-0.155}, & T_{ij}^* \ge 100 \end{cases}$
T_{ij}^*	=	$\frac{kT}{\varepsilon_{ij}}$
$\frac{\varepsilon_i}{k}$	=	Characteristic energy / Boltzmann's constant for gas i [K]
$\frac{\varepsilon_j}{k}$	=	Characteristic energy / Boltzmann's constant for gas j [K]
$\frac{\varepsilon_{ij}}{k}$	=	Characteristic energy / Boltzmann's constant for gas i and j [K]
	=	$\frac{1}{k}(\varepsilon_i\varepsilon_j)^{1/2}$

Chapman-Enskog, mix of low-pressure gases

$$\frac{1 - y_i}{D_{im}} = \sum_{j=1\neq i}^{m}\left(\frac{y_j}{D_{ij}}\right)$$

EOS

EOS a recently added MELCOR package with User Guide entry and input records

- Hydrodynamic condensable materials occupying either/or pool/atmosphere
- Backwards compatible with former methods (e.g. EXEC READFLUID)
- No required input for built-in water or single condensable via TPF and READFLUID
- Required input when multiple condensable hydrodynamic materials exist
- Interfaces closely with CVH and CVT and acts like a property library

EOS functions pervade the code:

- Touch points with COR, CVH, FL, and HS to permit multiple condensable fluids
- Packages specialized for water generate errors (BUR, CAV, CND, FCL, FDI, PAR, SPR)
- Special treatments, e.g. RN hygroscopic model and sensitivity coefficient sets

One default built-in (improved implementation for water), TPFs otherwise

EOS – Fluid Characterization

Require thermodynamic property functions:

- Pressure
- Entropy
- Internal energy
- Enthalpy
- Heat capacity at constant volume
- Heat capacity at constant pressure
- Compressibility
- Thermal expansion coefficient
- Isentropic sound speed

Properties a function of density and temperature (NCG – temperature only)

Fluids allowed to have two distinct phases: liquid and gas (NCG – gas only)

EOS – Property Libraries

Sodium properties/EOS based on SIMMER-III

MELEOS (user defined library) under development

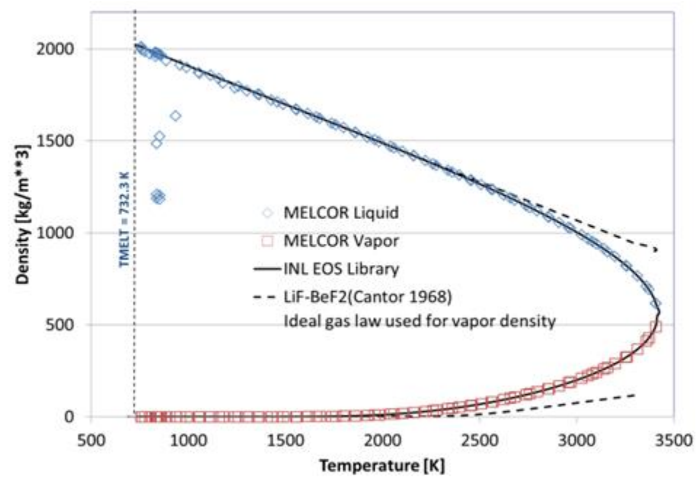
Multi-EOS facilitated by EOS package

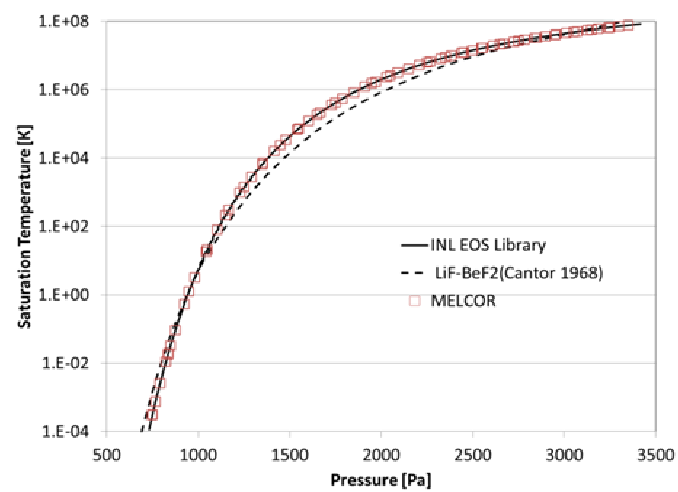
EOS implements properties/EOS from INL FSD

- Parametric Helmholtz Free Energy with 8 terms
- INL/CON-16-38063 on Pb-Li (Humrickhouse, Merrill)

Materials:

Fluid Name	Database Type	Database Name	Default File Name
Water	Built-in	Water	—
Water		H2O	tpfh2o
Hydrogen		H2	tpfh2
Lithium		Li	tpfli
Potassium		K	tpfk
Helium	TPF	He	tpfhe
Nitrogen		N2	tpfn2
Sodium		Na	tpfna
Sodium-Potassium		NaK	tpfnak
Lithium-Lead		LiPb	tpflipb
Fluoride-Lithium-Beryllium		FLiBe	tpffi





EOS – MELGEN Input

Define hydrodynamic condensable fluids and “EOS networks”

EOS_FLUID_ID – User Fluid Name and Sequence Number

Required

This record defines a unique, user-defined name for the fluid and a user-defined sequence number.

(1) EOS fluid name
(type = character*16, default = none)

(2) EOS fluid sequence number[2]
(type = integer, default = none)

Example

```
EOS_FLUID_ID 'Primary Fluid' 310
EOS_FLUID_ID Water 200
```

EOS_FLUID_TYPE – EOS Fluid Database Information

Required

This record defines the fluid that will be loaded into the problem. The first two fields are required for all fluids.

(1) EOS fluid database type
(a) BUILTIN
(b) TPF
(type = character*16, default = none)

(2) EOS fluid database name
Must be one of the database names are listed on Table 1.
(type = character*16, default = none)

The third field is only valid for TPF fluids and is optional:

(3) TPF Filename
(type = character*80, default = listed on Table 1)

```
eos_input

!   Fluids
eos_fluid_id     "primary"      1
eos_fluid_type   tpf    FLiBe
!
eos_fluid_id     Water      18
eos_fluid_type   Builtin      Water
!
eos_fluid_id     "eccs-2-fluid"     26
eos_fluid_type   tpf    Na     "na.tpf"
```

```
!   Networks
eos_network_id      "ECCS-Network"   51
eos_network_cv      "eccs-1"
eos_network_fluid   Water
!
eos_network_id      "Secondary-Network"    3
eos_network_cv      "eccs-2"
eos_network_fluid   "eccs-2-fluid"
!
eos_network_id      "Primary-Network"    498
eos_network_cv      "primary"
eos_network_fluid   "primary"
```

EOS_NETWORK_ID – User Network Name and Sequence Number

Required

This record defines a unique, user-defined name for the network and a user-defined sequence number.

(1) EOS network name
(type = character*16, default = none)

(2) EOS network sequence number
(type = integer, default = none)

Example

```
EOS_NETWORK_ID 'Primary' 310
EOS_NETWORK_ID Secondary 100
```

EOS_NETWORK_CV – EOS Network Control Volume

Required

This record gives the control volume name that will act as the starting point for the EOS network search, which is described in subsection 1.1 of this UG. If the control volume name does not exist or the control volume belongs to another EOS network, the code will generate an input processing error.

(1) Control Volume name
(type = character*16, default = none)

Example

```
EOS_NETWORK_CV 'Lower Head'
EOS_NETWORK_CV IRWST
```

EOS_NETWORK_FLUID – EOS Network Fluid

Required

This record gives the EOS fluid name that will be used to the select the EOS for the network. The EOS fluid name on this record must match one given on an EOS_FLUID_ID record or an input processing error will be issued.

(1) EOS fluid name
(type = character*16, default = none)

Example

```
EOS_NETWORK_FLUID 'Primary-fluid'
```

EOS – MELGEN Output

MELCOR

Display information about EOS and networks

- EOS processes/checks on MELGEN pass 2
- EOS package gives results of network accounting
  - Whether EOS package input invoked or not
  - Check work if explicitly specifying EOS networks
  - Information on CV/FL and HS surface association
- Confirms condensable fluid for each EOS network
  - Echo/confirm if EOS input invoked
  - “legacy EOS” otherwise, CVH confirming fluid

```
Diagnostics during PASS2 input processing CVH package:
*****USING FLUID NAMED = Flibe !*****
NO Errors during PASS2 input processing CVH package
```

- Coming soon…EOS data on fluids in output

```
  EOS Network Information
===========================
Number of Subnetworks: 3

  Network: Default Network 1
------------------------------
    ID:     1
    Fluid: Legacy EOS
    Control Volumes:
        - Distrib_100 (100)
            - Root CV
            - Connected to Annulus_105
            - Connected to ColdLeg_330
```

```
Diagnostics during MELGEN Pass 2 input processing of EOS package
INFO: created default EOS network not specified in input.
    Network named 'Default Network 1' with root CV 'Distrib_100'
INFO: created default EOS network not specified in input.
    Network named 'Default Network 2' with root CV 'Sec_in'
INFO: created default EOS network not specified in input.
    Network named 'Default Network 3' with root CV 'Dummy'
No Errors during MELGEN Pass 2 input processing of EOS package
```

```
ID:     2
Fluid: Legacy EOS
Control Volumes:
    - Sec_in (400)
        - Root CV
        - Connected to Sec_401
    - Sec_401 (401)
        - Connected to Sec_in
        - Connected to Sec_402
    - Sec_402 (402)
        - Connected to Sec_401
        - Connected to Sec_out
    - Sec_out (403)
        - Connected to Sec_402

Flow Paths:
    - Sec_400 (400)
        - Connected to Sec_in
        - Connected to Sec_401
    - Sec_401 (401)
        - Connected to Sec_401
        - Connected to Sec_402
    - Sec_402 (402)
        - Connected to Sec_402
        - Connected to Sec_out

Heat Structures Left Sides:
    - HXtube3200 (3200)
        - Convects to Sec_401
    - HXtube3211 (3211)
        - Convects to Sec_402

Heat Structures Right Sides:
    (None)
```

EOS – Liquid Freezing

Fusion system fluids tend to have relatively high T_{frz} vs. std room temperature

MELCOR 1.8.6 for fusion

- Anticipate fluids contact structures well below fluid's triple point
- Anticipate liquid freezing ("ice" formation) in control volume pools and in films on heat structures
- Extrapolate EOS at the triple point assuming constant fluid vapor or liquid density
  - Internal energy and pressure are functions of temperature and density
  - Derive extrapolated liquid/vapor internal energy and pressure as functions of triple point properties

MELCOR 2.X

- Supercooled pool model
- Liquid in a control volume pool not allowed to form a "solid phase" per se, but upon "freezing" hold the liquid as a "supercooled" pool
- Treatment applies to internal energy and allows calculations to continue when MELCOR and EOS would otherwise be unable

MELCOR 2.X vs. MELCOR 1.8.6 for Fusion

	Topic	M 2.X	M 1.8.6 fus	Comment
NCG Package	H_2 in default NCG library	YES	YES	M 1.8.6 may or may not have all options of M 2.X
	D_2 in default NCG library	YES	YES	-
	T_2 in default NCG library	NO	YES	User-definable in M 2.X
	HD in default NCG library	NO	YES	User-definable in M 2.X
	HT in default NCG library	NO	YES	User-definable in M 2.X
	DT in default NCG library	NO	YES	User-definable in M 2.X
	Dissolved Hydrogen Transport Model	NO	YES	Alternative approaches in M 2.X?
EOS Package	Liquid Metals			
	PbLi	YES	YES	TPF file via EOS in M 2.X
	Li	YES	YES	TPF file via EOS in M 2.X
	K	YES	YES	TPF file via EOS in M 2.X
	Na	YES	YES	TPF file via EOS in M 2.X
	NaK	YES	YES	TPF file via EOS in M 2.X
	SnLi	?	YES	Mentioned in MELCOR-TMAP discussions
	Molten salt (FLiBe)	YES	YES	TPF file via EOS in M 2.X
	Cryogenic Fluids			
	H2	YES	YES	TPF file via EOS in M 2.X
	He	YES	YES	TPF file via EOS in M 2.X
	N2	YES	YES	TPF file via EOS in M 2.X
	O2	?	YES	Mentioned in MELCOR-TMAP discussions
	Multiple condensable fluids allowed	YES	YES	Formulations differ but capabilities similar
	Liquid freezing	YES	YES	Formulations differ but capabilities similar

MELCOR 2.X Fluids Development

Add remaining hydrogen species (T_2, HD, HT, DT) to default NCG library

- Though they would be user-definable in MELCOR 2.X, somewhat burdensome
- Good idea to add even if a different approach is ultimately taken on hydrogen species

Procure/test TPF files for liquid metal SnLi and cryogenic fluid O_2 if necessary

- No expected difficulties or incompatibilities with MELCOR 2.X EOS package
- Any other condensable fluids for fusion systems missing?

Defer discussion of topics tangential to NCG and EOS

- Pool/atmosphere heat/mass transfer including dissolved species transport
- HTO transport
- Choked flow for non-light-water
- Liquid metal (CVH pool) convection heat transfer coefficients
- Liquid freezing within HS films
- Dispersed flow (as a departure from typical stratified flow)
- Magnetohydrodynamic pressure drop
- Lithium fires

Summary

Reviewed NCG equation-of-state methods

Reviewed EOS package concepts and inputs

Compared existing MELCOR 2.X fluids capabilities to MELCOR 1.8.6 for fusion

Suggested a small fluids-related development agenda for MELCOR 2.X