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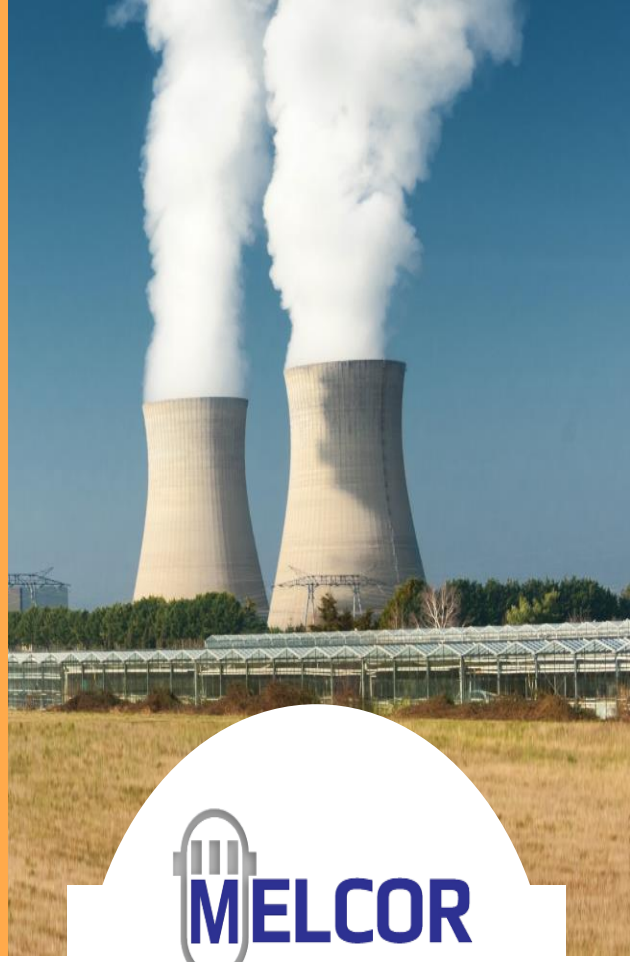


MELCOR

MELCOR 2.X for Fusion – HS Energy & Diffusion

2025 European MELCOR Users' Group Meeting

April 7th-11th, 2025

U.S.NRC

SAND2025-04010PE

Overview

Review

- MELCOR-TMAP (TMAP4 + MELCOR 1.8.6 for fusion)
- MELCOR HS energy/temperature solution
  - Heat conduction equation
  - Finite difference equation on the interior
  - Finite difference equation on the boundary

Proposed adaptation of TMAP HS diffusion modeling for MELCOR 2.X on HS

- Conservation statement
- Diffusive and thermophoretic fluxes
- Transport to and across a surface
- Nodalization, finite difference equation, and generalized interface flux on the interior
- Nodalization, finite difference equation, and surface flux on the boundary
- Pool and atmosphere interfacial heat/mass transfer

Summary

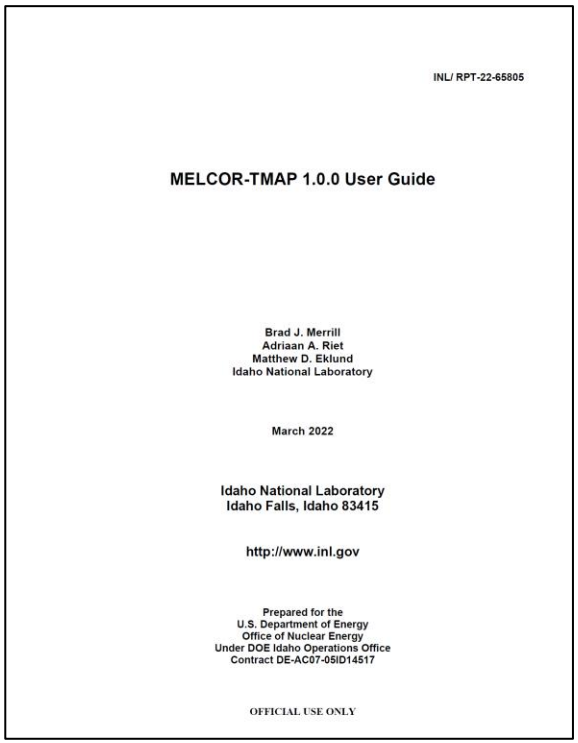
MELCOR-TMAP

INL FSP tasked with developing “fusion accident analysis tools required for licensing future U.S. fusion reactors”, and created MELCOR-TMAP accordingly

- Tritium Mitigation Analysis Program (TMAP)
  - Under development for decades
  - Physics:
    - Multi-species surface absorption
    - Dissolved gas (atomic or molecular) diffusion in/through composite materials including dislocation traps
    - Gas transport between structures and enclosures (gas spaces)
    - Own models for advection and transport between enclosures
- MELCOR 1.8.6 for fusion
  - Added new fluids
  - Added various fusion specific models/capabilities
- Integrated to create MELCOR-TMAP

MELCOR-TMAP

- TMAP physics models described in chapter 4 of UG →
- New MELCOR Input to inform integrated TMAP
  - HS surfaces (initial species concentrations, surface BC’s)
  - HS implanted species sources and trapping inputs
  - MP inputs – various (and many) new properties to inform diffusion calculations on HS of one or more materials



INL/ RPT-22-65805

MELCOR-TMAP 1.0.0 User Guide

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HS Energy/Temperature Solution

MELCOR HS package – see HS Users' Guide and Reference Manual

- HS conduction modeled with a heat conduction equation in one spatial dimension for many geometries

$$C_p \frac{\partial T}{\partial t} = \vec{\nabla} \cdot \left(k \vec{\nabla} T\right) + U$$

Where:

C_p = volumetric heat capacity (product of specific heat capacity at constant pressure and density) – $\left[{}^{J}/_{m^3} \right]$

T = temperature - $[K]$

U = volumetric power - $\left[{}^{W}/_{m^3} \right]$

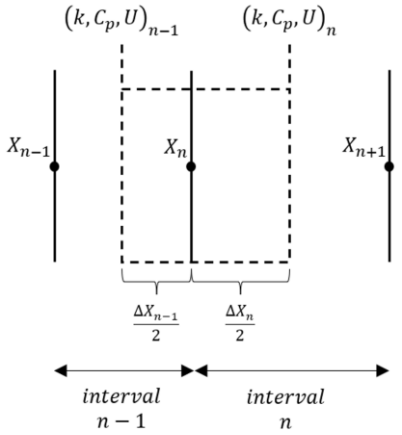
- Spatially partition structures into a number of temperature nodes
  - At boundary surfaces
  - At interfaces between materials within a structure
  - Arbitrarily within structure otherwise
- Region between two adjacent temperature nodes is called a mesh interval
- Mesh intervals of arbitrary thickness (i.e. arbitrary distance between adjacent nodes)
- Mesh intervals consist of a single material
- Control volumes of integration for finite difference equations relate to mesh intervals
  - CV interfaces located at mid-mesh interval, site of property information storage
  - CV "mid-points" are mesh interval interfaces, site of temperature information storage

TMAP diffusion solution occurs on same computational grid and is temperature dependent

HS Energy/Temperature Solution

Mesh intervals, nodes, CV of integration, and finite difference equations on HS interior

- About n^{th} node X_n on interior
- 2 mesh intervals: *n-1* and *n*
- 1 CV of integration
  - Left "half" part of interval *n-1*
  - Right "half" part of interval *n*
- Thermal properties and sources stored at CV interfaces (MI midpt)



N	=	number of temperature nodes in heat structure
n	=	interior node number (2, 3, …, N-1)
X	=	location of temperature node – $[m]$
ΔX_n	=	$X_{n+1} - X_n$, length of n^{th} mesh interval – $[m]$
k	=	thermal conductivity of material – $\left[{}^{W}/_{m*K}\right]$
C_p	=	volumetric heat capacity of material – $\left[{}^{J}/_{m^3}\right]$
U	=	volumetric power source – $\left[{}^{W}/_{m^3}\right]$

Integrate heat equation

$$\int_V \left(C_p \frac{\partial T}{\partial t}\right) dV = \int_V \left(\vec{\nabla} \cdot \left(k\vec{\nabla}T\right)\right) dV + \int_V (U)\, dV \longrightarrow \int_{V_L} \left(C_{p,L} \frac{\partial T}{\partial t}\right) dV + \int_{V_R} \left(C_{p,R} \frac{\partial T}{\partial t}\right) dV = \int_V \left(\vec{\nabla} \cdot \left(k\vec{\nabla}T\right)\right) dV + \int_{V_L} (U_L)\, dV + \int_{V_R} (U_R)\, dV$$

Apply divergence theorem, carry out volume integrations, and apply time-differencing

$$\int_V \left(\vec{\nabla} \cdot \left(k\vec{\nabla}T\right)\right) dV = \int_S \left(\hat{n} \cdot \left(k\vec{\nabla}T\right)\right) dA \longrightarrow \left(\left(C_{p,L}\Delta V_L\right) + \left(C_{p,R}\Delta V_R\right)\right)\left(\frac{T_n^m - T_n^{m-1}}{\Delta t}\right) = A_R\left(k\vec{\nabla}T\right)_R - A_L\left(k\vec{\nabla}T\right)_L + (U_L)\Delta V_L + (U_R)\Delta V_R$$

Approximate unknown flux terms (Fourier's law)

$$\left(\left(C_{p,L}V_L\right) + \left(C_{p,R}V_R\right)\right)\left(\frac{T_n^m - T_n^{m-1}}{\Delta t}\right) = A_R k_n \left(\frac{T_{n+1}^m - T_n^m}{\Delta X_n}\right) - A_L k_{n-1}\left(\frac{T_n^m - T_{n-1}^m}{\Delta X_{n-1}}\right) + (U_L)V_L + (U_R)V_R$$

Define "left" and "right" surface (HSL, HSR) and volume (HVL, HVR) "weights"

$$\left(C_{p,n-1}HVL_n + C_{p,n}HVR_n\right)\left(\frac{T_n^m - T_n^{m-1}}{\Delta t_m}\right) = HSR_n k_n (T_{n+1}^m - T_n^m) + HSL_n k_{n-1}(T_{n-1}^m - T_n^m)$$

HS Energy/Temperature Solution

Surface and volume weights on the interior

- Various definitions pending geometry
- Surface weight
  - Outworking of divergence theorem and CV int flux
  - 1-D interpretation of “area” divided by interval width
- Volume weight
  - Outworking of volume integration
  - Mesh interval “half-volume”…1-D “volume”

Cartesian

- “1-D surf areas” evaluate to unity
- “1-D volumes” evaluate to slab volume per length

Cylindrical

- “1-D surf areas” are a circumference
- “1-D volumes” are cylindrical shell vol per length

Spherical/hemispherical

- “1-D surf areas” are spherical shell surface areas
- “1-D volumes” are spherical shell volumes

HS Geometry		Weight Units
Rectangular	$HSL_n = 1/\Delta X_{n-1}$	m^{-1}
	$HVL_n = \Delta X_{n-1}/2$	m
	$HSR_n = 1/\Delta X_n$	m^{-1}
	$HVR_n = \Delta X_n/2$	m
Cylindrical	$HSL_n = 2\pi\left(X_n - \frac{\Delta X_{n-1}}{2}\right)/\Delta X_{n-1}$	–
	$HVL_n = \pi\left(X_n^2 - \left(X_n - \frac{\Delta X_{n-1}}{2}\right)^2\right)$	m^2
	$HSR_n = 2\pi\left(X_n + \frac{\Delta X_n}{2}\right)/\Delta X_n$	–
	$HVR_n = \pi\left(\left(X_n + \frac{\Delta X_n}{2}\right)^2 - X_n^2\right)$	m^2
Spherical	$HSL_n = 4\pi\left(X_n - \frac{\Delta X_{n-1}}{2}\right)^2/\Delta X_{n-1}$	m
	$HVL_n = \frac{4\pi}{3}\left(X_n^3 - \left(X_n - \frac{\Delta X_{n-1}}{2}\right)^3\right)$	m^3
	$HSR_n = 4\pi\left(X_n + \frac{\Delta X_n}{2}\right)^2/\Delta X_n$	m
	$HVR_n = \frac{4\pi}{3}\left(\left(X_n + \frac{\Delta X_n}{2}\right)^3 - X_n^3\right)$	m^3

HS Energy/Temperature Solution

Mesh intervals, nodes, CV of integration, and finite difference equations on HS boundary

- Path bifurcates based on absence/presence of a liquid film
- If liquid film absent:
  - No extra mesh intervals created, no extra equations for the heat structure
  - Apply a boundary condition to calculate surface temperature
- If liquid film present:
  - Create additional film mesh interval(s) (bound inside by HS surface, bound outside by interfacial node)
  - Extra equation for the liquid film
  - Particular form of a convective heat/mass transfer boundary condition applied at film/atmosphere interface

Generic boundary condition

- Implicit in surface temperature
- Derive any particular condition
  - Symmetry (adiabatic)
  - Convective
  - Specified flux or specified temperature

$$\alpha T + \beta \frac{dT}{dN} = \gamma$$

Where:

α	=	first boundary condition coefficient
β	=	second boundary condition coefficient
γ	=	third boundary condition coefficient
T	=	surface temperature (collocated with a temperature node)
$\frac{dT}{dN}$	=	gradient of temperature along outward normal from surface

Back-up slides outline boundary nodalizations and finite difference equations

TMAP Adapted for HS

MELCOR

Elements of transport theory:

- Conservation – Solute (atomic or molecular gas) species *s* transports as:

$$\frac{\partial C_s}{\partial t} = -\left(\vec{\nabla} \cdot \vec{J_s}\right) + S_s - \frac{\partial C_s^t}{\partial t}$$

Where:

C_s = Concentration of atomic species s [atom|molecule/m^3]

$\vec{J_s}$ = Flux of species s atoms [atom|molecule/m^2/s]

S_s = Source (production rate) of species s [atom|molecule/m^3/s]

C_s^t = Concentration of trapped species s [atom|molecule/m^3]

- Diffusive and Thermophoretic Flux for solute species *s* is generally:

$$\vec{J_s} = -D_s\left(\vec{\nabla} C_s + \left(\frac{Q_s^* C_s}{RT^2}\right)\left(\vec{\nabla} T\right)\right)$$

Where:

D_s = Diffusivity (diffusion coefficient) of atomic species s in structure [m^2/s]

Q_s^* = Heat of transport [J/mol] of Ludwig-Soret coefficient, atomic species s

R = Universal gas constant = 8.314 [J/mol/K]

T = Local structural temperature [K]

TMAP Adapted for HS

Elements of transport theory:

- Trapping and Release
  - Trap sites effectively increase energy required to move through material (relative to pure diffusion)
  - Could result from impurities or structural irregularities (e.g. cold working or neutron fluence)
  - Mathematically modeled as:

$$\frac{\partial C_{s,j}^{t}}{\partial t} = \frac{\alpha_{t,s} C_{j,t}^{e}}{N} C_s - \alpha_{r,j} C_{s,j}^{t}$$

$$C_{j,t}^{e} = C_{j,t}^{o} - \sum_{s=1}^{N_s} \left(C_{s,j}^{t} \right)$$

$$\alpha_{t,s} = \frac{D_s}{\lambda^2}$$

$$\alpha_{r,j} = v_0 e^{\left[-E_{j,t} / k_{BC} T \right]}$$

Where:

$C_{s,j}^{t}$	= Concentration of trapped species s [atom|molecule/m^3] in trap site j
$C_{j,t}^{o}$	= Concentration of trap sites, type j [1/m^3], sum of occupied and empty sites
$C_{j,t}^{e}$	= Concentration of empty trap sites, type j [1/m^3]
λ	= Jump distance, usually the lattice constant [m]
v_0	= Release attempt frequency, usually the Debye frequency ~ 10^{13} [1/s]
$E_{j,t}$	= Trapping energy [eV], diffusion activation plus binding energies of trap site type j
N	= Atomic number density [atom/m^3] of host (heat structure) material
N_s	= Total number of solute species s
$\alpha_{t,s}$	= Trapping rate coefficient [1/s] for species s
$\alpha_{r,j}$	= Release rate coefficient [1/s] for all species from trap site type j

- Trapping source term for species s is a sum over N_T total trap site types j
- Trapping functions as a source term in conservation equation

TMAP Adapted for HS

Elements of transport theory:

- Transport to/across a surface
  - Gas movement across a surface mathematically described depending on material
  - If metal, gas molecules dissociate, transport in solution as atomic gas, and must recombine upon exit (Sievert)
  - If non-metal, gas molecules do not dissociate but transport through material and exit in same form (Henry)
- Sievert's law and Sievert's solubility coefficient
  - Rule for solubility of diatomic gas in metal
  - Depends on partial pressure in equilibrium (above surface)

$$C_i = K_s P_m^{1/2}$$

Where:

K_s = Sievert's law solubility coeffiecient [atom /m^3/Pa$^{1/2}$]

C_i = Surface concentration [atom/m^3] of atomic species i

P_m = Partial pressure [Pa] of molecular species m - containing species i

- Henry's law and Henry's solubility coefficient
  - Rule for solubility of gas in non-metal
  - Depends on partial pressure (above surface)

$$C_m = K_h P_m$$

Where:

K_h = Henry's law solubility coefficient [atom /m^3/Pa]

C_m = Surface concentration [atom/m^3] of molecular species m

P_m = Partial pressure [Pa] of molecular species m above surface

TMAP Adapted for HS

Elements of transport theory:

- Transport to/across surface –Sievert's or Henry's law – formulated with mass transport coefficients

$$\Gamma_i = -K_{T,i}\left(C_{B,i} - C_{S,i}\right)$$

Where:

$C_{B,i}$ = Bulk concentration [atom/m^3] of species i

$C_{S,i}$ = Surface concentration [atom/m^3] of species i

$K_{T,i}$ = Mass transfer coefficient [m/s] for species i

- Mass transport coefficients ascertained from heat/mass transfer analogy

$$\frac{K_{T,i}}{\rho_l D_{i,l}} = \frac{h_l}{k_l}\left(\frac{Sc}{Pr}\right)^{1/3}$$

Where:

Pr = Liquid l Prandtl number = $\left(\mu_l c_{p,l}\right)/k_l$

Sc = Liquid l Schmidt number = $\mu_l/\left(\rho_l D_{i,l}\right)$

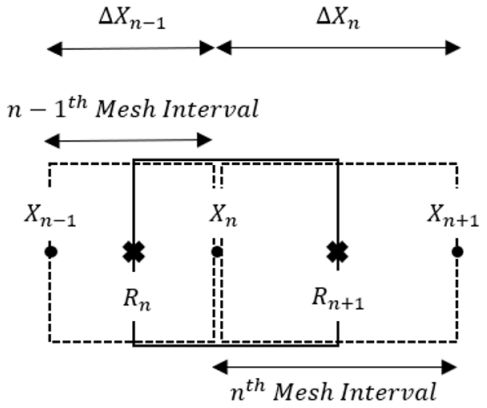
h_l = Liquid heat transfer coefficient = $0.02\rho_l c_{p,l} v_l$

- Computational nuances entailed in the bulk vs surface concentrations
  - Sievert's condition to describe equilibrium given the dissociation/recombination complication
    - Bulk atmosphere of multiple mixed-atomic gases, and surface with dissociated atomic gas species
    - Chemical equilibrium condition applied
  - Henry's condition more straightforward in describing relationship between bulk and surface
- Use mass transport coefficient approach when describing mass transfer from pool

TMAP Adapted for HS

Nodalization and control volume of integration on interior

- Diffusion CVs of integration are staggered with respect to energy/temperature CVs
- Diffusion CVs coincide with HS mesh intervals (material transitions at CV interfaces)
- Diffusion coefficients and property information stored where concentrations known



DIFF CV

E/T CV

- T node, DIFF CV interface

✖ C node, Energy/Temperature CV interface and mid mesh interval

Where:

X	=	location of temperature node
R	=	location of concentration node
ΔX_n	=	$X_{n+1} - X_n$, length of n^{th} heat structure mesh interval

- Integrating, applying divergence theorem, and writing in terms of unknown diffusion fluxes:

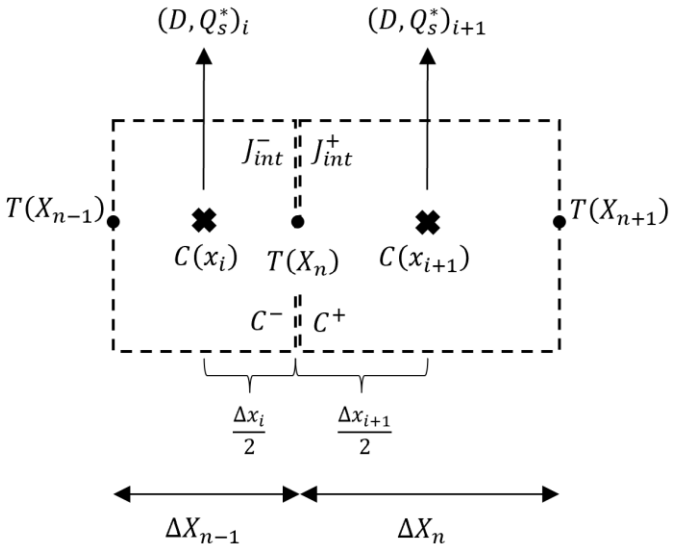
$$\int_V \left(\frac{\partial C_s}{\partial t}\right) dV = -\int_V \left(\vec{\nabla} \cdot (\vec{J}_s)\right) dV + \int_V (S_s)\, dV - \int_V \sum_{j=1}^{N_T} \left(\frac{\partial C_s^t}{\partial t}\right) dV \longrightarrow \left(\frac{\partial C_s}{\partial t}\right) \Delta V_i = A_R (J_s)_R - A_L (J_s)_L + (S_s)\Delta V_i - \left(\sum_{j=1}^{N_T} \left(\frac{\partial C_s^t}{\partial t}\right)\right) \Delta V_i$$

- Require a general relationship for unknown interface flux terms

TMAP Adapted for HS

Generalized interface flux relationship (accommodate any condition at interface)

- Flux continuity enforces: $J^{-}_{s,int} = J^{+}_{s,int} = J_{s,int}$
- Derive a general expression for $J_{s,int}$
- Complicated derivation especially given thermophoretic term
  - Write expression for $J^{-}_{s,int}$ and $J^{+}_{s,int}$
  - Use space-centered differencing on gradient terms
  - Apply a generic partition coefficient condition: $\gamma_s C^{+}_s = C^{-}_s$
  - Do a lot of algebra and arrive at: $J_{s,int} = -G_i\left(C_{s,i} - \chi_i C_{s,i+1}\right)$



$$G_i = \frac{dx_i dx_{i+1} F^{+}_{s,i} F^{+}_{s,i+1}}{\gamma_{s,i} dx_i F^{-}_{s,i} + dx_{i+1} F^{+}_{s,i+1}} \qquad \chi_i = \frac{\gamma_{s,i} F^{-}_{s,i} F^{-}_{s,i+1}}{F^{+}_{s,i} F^{+}_{s,i+1}}$$

$$\Delta T_i = T_i - T_n \qquad \Delta T_{i+1} = T_n - T_{i+1}$$

$$dx_i = \frac{1}{\Delta x_i/2} = \frac{2}{\Delta x_i} \qquad dx_{i+1} = \frac{1}{\Delta x_{i+1}/2} = \frac{2}{\Delta x_{i+1}}$$

$$F^{+|-}_{s,i|i+1} = D_{s,i|i+1}(+|-)A_{s,i|i+1}\Delta T_{i|i+1} = \begin{cases} F^{+}_{s,i} = D_{s,i} + A_{s,i}\Delta T_i \\ F^{-}_{s,i} = D_{s,i} - A_{s,i}\Delta T_i \\ F^{+}_{s,i+1} = D_{s,i+1} + A_{s,i+1}\Delta T_{i+1} \\ F^{-}_{s,i+1} = D_{s,i+1} - A_{s,i+1}\Delta T_{i+1} \end{cases}$$

- applying, time-differencing, and manipulating the trapping term:

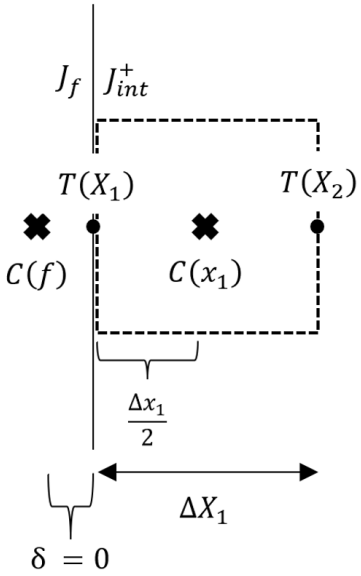
$$\left(\frac{C^{m}_{s,i} - C^{m-1}_{s,i}}{\Delta t}\right)\Delta V_i = A_R\left(\chi_i G_i C_{s,i+1} - G_i C_{s,i}\right) - A_L\left(\chi_{i-1} G_{i-1} C_{s,i} - G_{i-1} C_{s,i-1}\right) + (S_s)\Delta V_i - \left(\sum_{j=1}^{N_T}\left(\frac{\left(\frac{C^{t,m-1}_{s,i,j} + \frac{\alpha_{t,s,i}}{N}\left(C^{e}_{i,j,t}\right)^m}{1 + \alpha_{r,i,j}\Delta t}\right) C^{m}_{s,i}\Delta t - C^{t,m-1}_{s,i,j}}{\Delta t}\right)\right)\Delta V_i$$

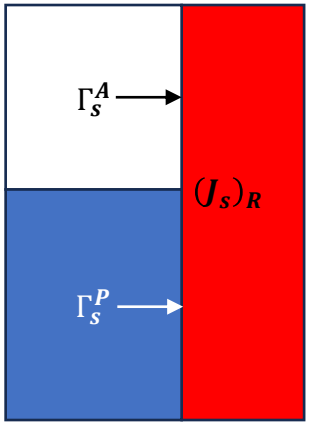
HS Geometry		Units
Rectangular	$A_L = 1$	–
	$A_R = 1$	–
	$\Delta V_i = \Delta X_i/2$	m
Cylindrical	$A_L = 2\pi X_i$	m
	$A_R = 2\pi X_{i+1}$	m
	$\Delta V_i = \pi\left({X_{i+1}}^2 - X_i^2\right)$	m^2
Spherical	$A_L = 4\pi(X_i)^2$	m^2
	$A_R = 4\pi(X_{i+1})^2$	m^2
	$\Delta V_i = \frac{4\pi}{3}\left(X^3_{i+1} - X^3_i\right)$	m^3
Hemispherical	$A_L = 2\pi(X_i)^2$	m^2
	$A_R = 2\pi(X_{i+1})^2$	m^2
	$\Delta V_i = \frac{2\pi}{3}\left(X^3_{i+1} - X^3_i\right)$	m^3

TMAP in Modern MELCOR

Nodalization and control volume of integration on boundary

- Zero-thickness diffusion CV at surface
- Essentially imposes a flux (interface) condition on 1st diffusion CV in material
- Conservation equation is a simple flux balance: $A_R(J_s)_R = A_L(J_s)_L$
  - Areas are equal on either side of the zero-thickness boundary CV
  - Right-hand flux can be written as: $(J_s)_R = C_{s,1}dr_1F_{s,1}^- - C_{s,f}dr_1F_{s,1}^+$
  - Left-hand flux can be written according to condition of choice
    - Zero-flux
    - Specified surface concentration (constant or some functional dependence)
    - Mass transport coefficient condition: $(J_s)_L = (1-\omega)\Gamma_s^A + (\omega)\Gamma_s^P$
      - Surface/pool component – MTC with Henry's/Sievert's law
      - Surface/atmosphere component – recombination/dissociation
      - Heavy solution law dependence





$$J_i = \sum_{m=1}^{N_s}\left(n_i^m K_{d_m} P_m\right) - 2\sum_{j=1}^{N_s}\left(K_{r,ij} C_i C_j\right)$$

Where:

J_i = Atomic gas species i flux [atom /m^2/s] into surface

n_i^m = number of atoms of species i in molecule of species m

K_{d_m} = Dissociation coefficient [1/Pa/m^2/s] for molecular species m consisting of species i and j

$K_{r,ij}$ = Recombination coefficient [m^4/s] for molecular species m consisting of species i and j

$C_{i|j}$ = Surface concentration [atom/m^3] of atomic species i or j

$$\Gamma_s^A = \sum_{m=1}^{N_m}\left(n_i^m K_{d,m} P_m\right) - 2\sum_{j=1}^{N_s}\left(K_{r,i,j} C_{f,i} C_{f,j}\right)$$

TMAP in Modern MELCOR

Pool surface heat/mass transfer

- 6 hydrogen molecules in pool/atm (H_2, D_2, T_2, HD, HT, DT) and 3 isotopes in solid phase (H, D, T)
- MELCOR-TMAP treated hydrogen species with NCG (components of atmosphere)
- MELCOR-TMAP had specialized conservation equations for (dissolved) hydrogen species in pool
- Treats hydrogen species as "trace" contaminants
- Take account of:
  - Generation in pool (user-defined)
  - Pool surface transfer
    - Mass transport coefficient

$$\Gamma_i = -K_{T,i}\left(C_{B,i} - C_{S,i}\right)$$

Where:

$C_{B,i}$ = Bulk concentration [atom/m^3] of species i

$C_{S,i}$ = Surface concentration [atom/m^3] of species i

$K_{T,i}$ = Mass transfer coefficient [m/s] for species i

$$\frac{K_{T,i}}{\rho_l D_{i,l}} = \frac{h_l}{k_l}\left(\frac{Sc}{Pr}\right)^{1/3}$$

Where:

Pr = Liquid l Prandtl number = $\left(\mu_l c_{p,l}\right)/k_l$

Sc = Liquid l Schmidt number = $\mu_l/\left(\rho_l D_{i,l}\right)$

h_l = Liquid heat transfer coefficient = $0.02\rho_l c_{p,l} v_l$

  - Outgassing: $\frac{\partial C_{B,i}}{\partial t} = \frac{A_p \Gamma_i}{V_p}$

Where:

A_p = Pool surface area [m^2]

V_p = Pool volume [m^3]

  - HS surface transfer (discussed previously)

Summary

Reviewed the energy/temperature derivation for HS as a lead-in to diffusion

Reviewed theory useful to hydrogen transport modeling

Reviewed aspects of the finite difference equations for hydrogen transport in HS

- Expect this formulation would be generalized for arbitrary species transport
- Math much simpler without:
  - Thermophoretic component of flux
  - Trapping/release

Reviewed MELCOR-TMAP treatment of hydrogen species transport in CV pol/atm

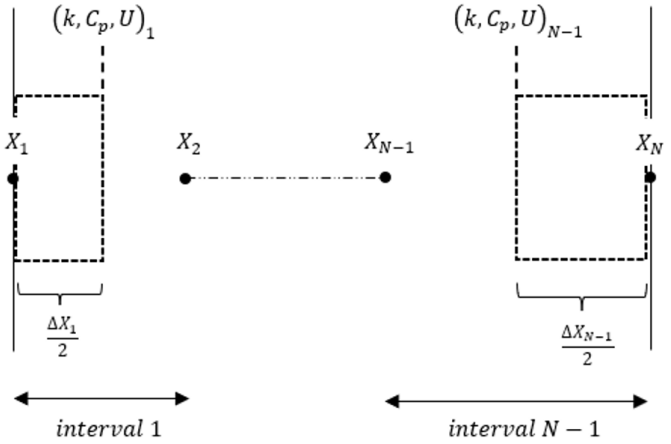
- Pool bulk to pool/atmosphere surface
- Pool/atmosphere to/from HS surfaces
- Atmosphere from pool/atmosphere surface

Backup Slides

Backup – Energy Solution on Boundary

Mesh intervals, nodes, CV of integration, and finite difference equations on HS boundary

Treatment depends upon whether a liquid film exists…if no liquid film:



$$\int_{V_R}\left(C_{p,R}\frac{\partial T}{\partial t}\right)dV = A_R\left(k\vec{\nabla}T\right)_R - A_L\left(k\vec{\nabla}T\right)_L + \int_{V_R}(U_R)\,dV$$

$$\downarrow$$

$$\left(C_{p,R}V_R\right)\left(\frac{T_1^m - T_1^{m-1}}{\Delta t}\right) = A_R k_1\left(\frac{T_2^m - T_1^m}{\Delta X_1}\right) - A_L\left(k\vec{\nabla}T\right)_L + (U_R)V_R$$

Generic boundary condition inform surface flux term: $A_L\left(k\vec{\nabla}T\right)_L = A_L k_1\frac{dT}{dr} = A_L k_1\left(-\frac{dT}{dN}\right) = A_L\left(\frac{-k_1}{\beta_L}\right)(\gamma_L - \alpha_L T_1)$

Finite difference equations:

$$(G_1)\left(\frac{T_1^m - T_1^{m-1}}{\Delta t_m}\right) = HSR_1 k_1(T_2^m - T_1^m) + HSL_1\left(\frac{k_1}{\beta_L}\right)(\gamma_L - \alpha_L T_1) + (U_1)HVR_1 \qquad G_1 = C_{p,1}HVR_1$$

$$(G_{N-1})\left(\frac{T_{N-1}^m - T_{N-1}^{m-1}}{\Delta t_m}\right) = HSL_{N-1}k_{N-1}(T_N^m - T_{N-1}^m) + HSR_{N-1}\left(\frac{\kappa_{N-1}}{\beta_R}\right)(\gamma_R - \alpha_R T_N) + (U_{N-1})HVL_{N-1} \qquad G_{N-1} = C_{p,N-1}HVL_{N-1}$$

Special term for evaporating film (not draining film):

$$-\frac{m_{f.L}^m \Delta h_{f,L}}{f} \qquad -\frac{m_{f.R}^m \Delta h_{f,R}}{f}$$

Where:

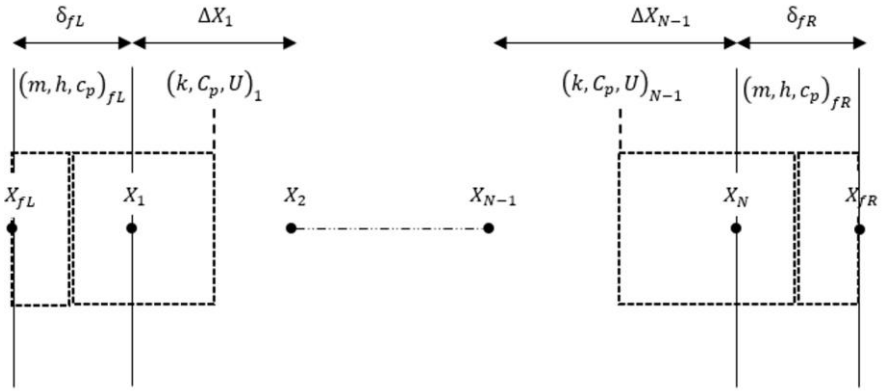
$m_{f,L|R}^m$ = old-time level m mass of film evaporated (or transferred) in Δt_m

$\Delta h_{f,L|R}$ = specific enthalpy added to $m_{f,L|R}^m$ before removal = $\begin{cases}\Delta h_{fg}, vaporizing \\ 0, draining\end{cases}$

Backup – Energy Solution on Boundary

Mesh intervals, nodes, CV of integration, and finite difference equations on HS boundary

Treatment depends upon whether a liquid film exists…if liquid film:



$\delta_{f,L|R}$ = thickness of liquid film at left or right surface

$m_{f,L|R}$ = mass of liquid film at left or right surface

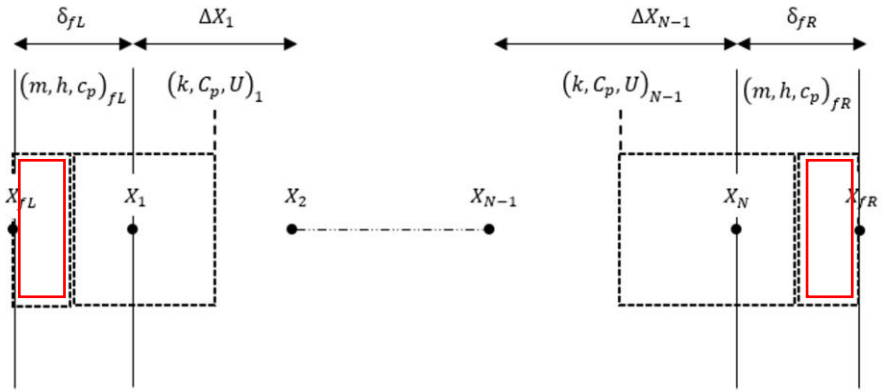
$h_{f,L|R}$ = specific enthalpy of liquid film at left or right surface

$C_{pf,L|R}$ = specific heat of liquid film at left or right surface

- Keep structure surface temperature node at original location
- Extra film temperature node (film/atmosphere interface), extra film mesh interval, 2 CVs of integration:
  - Liquid film mesh interval half-width
  - Surface CV with other liquid film mesh interval half-width plus 1st structural mesh interval half-width
  - Execute integration over each, and both entail some special treatment
- Assume no energy generation in the film mesh interval, but generally allow energy generation in structure
- Apply specially-crafted convection conditions on either interface of the film mesh interval half-width CV
- Apply specially-crafted convection condition on the outer interface of the film/structure CV
- Where the film/atmosphere interface is above pool, allow for condensation/evaporation

Backup – Energy Solution on Boundary

Boundary CV of film mesh interval half-width



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$$\int_{V_R}\left(C_{p,R}\frac{\partial T}{\partial t}\right)dV = A_R\left(k\vec{\nabla}T\right)_R - A_L\left(k\vec{\nabla}T\right)_L$$

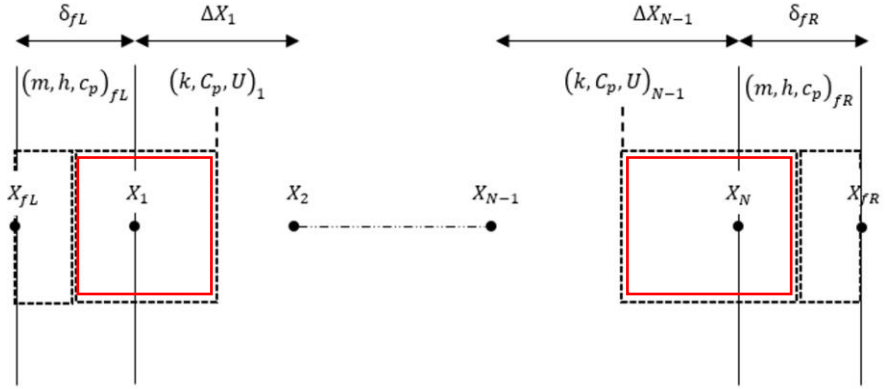
$$\begin{cases} A_L\left(k\vec{\nabla}T\right)_L = A_L k_{fL}\dfrac{dT}{dr} = A_L k_{fL}\left(-\dfrac{dT}{dN}\right) = A_L\left[\left(h_{atm,L}+h_{atmr.L}\right)\left(1-x_{pool,L}\right)\left(T_{fL}-T_{atm,L}\right)\right. \\ \qquad\qquad \left. + h_{pool,L}x_{pool,L}\left(T_{fL}-T_{pool,L}\right)\right] \\ A_R\left(k\vec{\nabla}T\right)_R = A_R k_{fL}\dfrac{dT}{dr} = A_R k_{fL}\left(\dfrac{dT}{dN}\right) = A_R\left[h_{fL}\left(T_1-T_{fL}\right)\right] \end{cases}$$

Finite difference equation accounting for condensation/evaporation mass flux:

$$\begin{aligned} &\left(G_{fL}\right)\left(\frac{T_{fL}^{m}-T_{fL}^{m-1}}{\Delta t_m}\right) \\ &\quad = HSR_{fL}\left[h_{fL}\left(T_1-T_{fL}\right)\right] \\ &\quad + HSL_{fL}\left[\left(h_{atm,L}+h_{atmr.L}\right)\left(1-x_{pool,L}\right)\left(T_{atm,L}-T_{fL}\right)\right. \\ &\quad \left. + h_{pool,L}x_{pool,L}\left(T_{pool,L}-T_{fL}\right)\right] \\ &\quad + \left[\left(1-x_{pool,L}\right)\left(\frac{A_L}{f}\right)\right]\left[\left(h_{v,L}-e_{f,L}\right)*MAX\left(0,\dot{m}_{C,L}\right)\right] \longrightarrow \textbf{Condensation} \\ &\quad + \left[\left(1-x_{pool,L}\right)\left(\frac{A_L}{f}\right)\right]\left[\left(h_{v,L}-\bar{e}_{f,L}\right)*MIN\left(0,\dot{m}_{C,L}\right)\right] \longrightarrow \textbf{Evaporation} \end{aligned}$$

Backup – Energy Solution on Boundary

Boundary CV of film mesh interval half-width and structural mesh interval half-width



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$$\left(\left(C_{p,L}\Delta V_L\right)+\left(C_{p,R}\Delta V_R\right)\right)\left(\frac{T_n^m-T_n^{m-1}}{\Delta t}\right)=A_R\left(k\vec{\nabla}T\right)_R-A_L\left(k\vec{\nabla}T\right)_L+\left(U_L\right)\Delta V_L+\left(U_R\right)\Delta V_R$$

Convection **0**

Spatial Differencing

Finite difference equation allowing condensation but disallowing evaporation (inside of film)

$$\begin{aligned}&\left(G_{fL}+G_1\right)\left(\frac{T_1^m-T_1^{m-1}}{\Delta t_m}\right)\\&\quad=HSR_1k_1(T_2-T_1)-HSR_{fL}h_{fL}\left(T_1-T_{fL}\right)\\&\quad+\left[\left(1-x_{pool,L}\right)\left(\frac{A_L}{f}\right)\right]\left[\left(e_{f,L}-\bar{e}_{f,L}\right)*MAX\left(0,\dot{m}_{C,L}\right)\right]\\&\quad+U_1HVR_1\end{aligned}$$

→ **Condensation above pool level**
No evaporation allowed