Moisture Diffusion Modeling with ANSYS at R14 and Beyond

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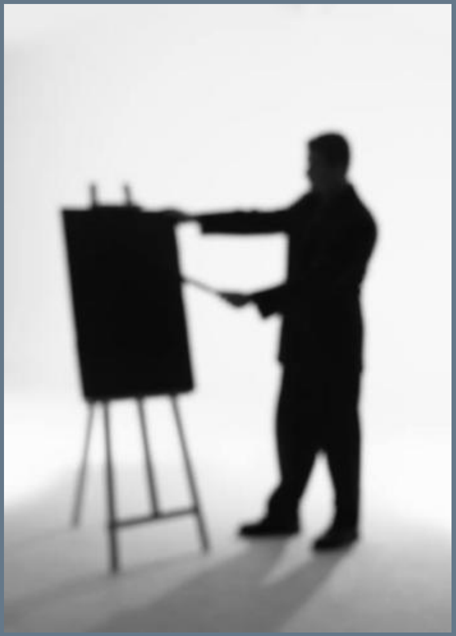
Phoenix Analysis & Design Technologies

Agenda

- Coupled-diffusion at 14.0
- Standard diffusion at 14.5
- Electromigration and other coupled-diffusion applications at 15.0 and Beyond



Things change, so don't hold me to stuff beyond 14.0

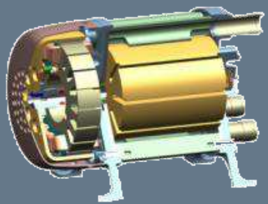
Introductions

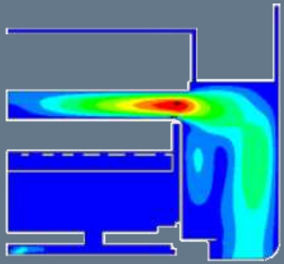
Upcoming Webinars

- Upcoming Webinars
  - ~~*Feb 9, 2012 - 12:00 MST*~~
    ~~**Working Directly with Nodes and Elements in ANSYS Mechanical**~~
  - ~~*Feb 23, 2012 - 12:00 MST*~~
    ~~**Assembly Meshing in ANSYS R14 CANCELED**~~
  - ~~*March 8, 2012 - 12:00 MST*~~
    ~~**Intro to Workbench Framework Scripting - Controlling projects, materials, and solution execution with python**~~
  - ~~*March 22, 2012 - 12:00 MST*~~
    ~~**Mastering the Remote Solver Manager (RSM) at R14**~~
  - ~~*April 12, 2012 – 12:00 MST*~~
    ~~**A POST26 Primer: Post Processing over Multiple Time/Load Steps in Mechanical APDL**~~
  - ~~April 26, 2012 – 12:00 MST~~
    ~~**A Constraint Equation Primer: How to Tie Degrees of Freedom Together**~~
  - ~~May 10, 2012 – 12:00 MST~~
    ~~**Optimization with ANSYS DesignXplorer at R14**~~
  - ~~May 24, 2012 – 12:00 MST~~
    ~~**Modeling Moisture Diffusion in ANSYS**~~
  - **Summer Break: June & July** (maybe August) (It is way too hot to do these things…)
- See upcoming and past webinars at:
  - padtincevents.webex.com
    - Click on ANSYS Webinar Series

About PADT

- PADT is an Engineering Services Company
  - Mechanical Engineering
  - 18 Years of Growth and Happy customers
  - 70'ish Employees
- 3 Business Areas
  - CAE Sales & Services
    - Consulting, Training, Sales, Support
  - Product Development
  - Rapid Prototyping & Manufacturing
- Learn More: www.PADTINC.com





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    96 Cores / 512 GB RAM / 6 TB Disk
    Mobile Rack / UPS / Monitor / Keyboard
    $34,900
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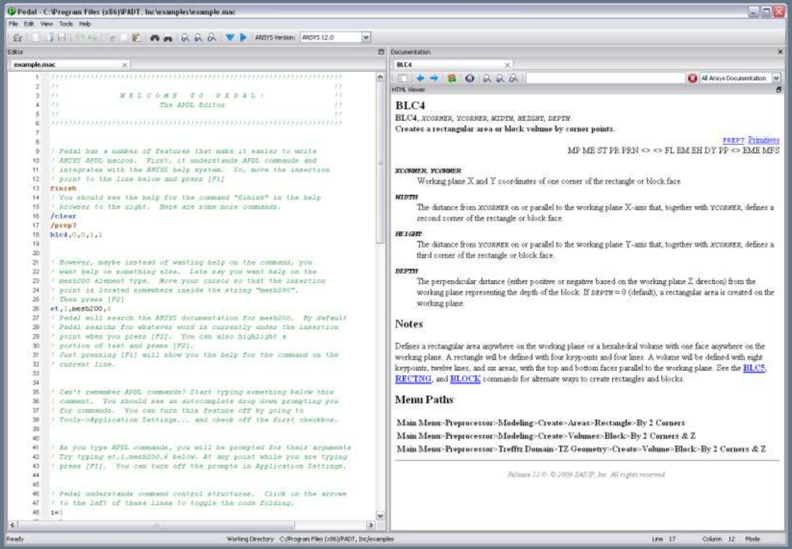
  - **Simulation Workstation (AMD)**
    12 Cores / 64 GB RAM / 3 TB Disk
    $6,300
- www.CUBE-HVPC.com

Cores	96 (2x4x12)	48 (4x12)	32 (4x8)	16 (2x8)	12 (2x6)	6 (1x6)	Fileserver (2x8)
System Name	c96SEi	c48	c32	w16	w12	w6	fs10
Price	$43,250	$15,500	$12,300	$11,600	$5,800	$5,400	$5,800
Configuration	2 x 2U Rack	1U Rack	1U Rack	Tower	Tower	Tower	2U Rack
CPU	2.3GHz AMD 6176	2.3GHz AMD 6176	2.4GHz AMD 6136	2.6GHz AMD 6140	2.8GHz AMD 4184	2.8GHz AMD 4184	2.0GHz AMD 6128
RAM (DDR3 1333)	256GB	128GB	128GB	128GB	64GB	32GB	16GB
OS Drive	256 GB SSD	256 GB SSD	256 GB SSD	256 GB SSD	256 GB SSD	320 GB Hybrid	-
Data Drives	3.6 TB 6 x 600 GB SAS2 15k RAID0	3 TB 3 x 1 TB 7.2K SATAII RAID0	3 TB 3 x 1 TB 7.2K SATAII RAID0	1.7 TB 3 x 600GB SAS2 15k RAID0	1.5TB 3 x 500 GB 7.2K SATAII RAID0	1.5TB 3 x 500 GB 7.2K SATAII RAID0	10 TB 8 x 1.5 TB 7.2K SATAII RAID60
NIC	2 x GigE	2 x GigE	2 x GigE	4 x GigE	2 x GigE	2 x GigE	2 x GigE
Video Card	Matrox 16MB	Matrox 16MB	Matrox 16MB	QuadroFX 580	QuadroFX 580	QuadroFX 580	Matrox 16MB
OS	CentOS Linux64	CentOS Linux64	CentOS Linux64	Windows 7 64	Windows 7 64	Windows 7 64	CentOS Linux64
Infiniband	QDR 40Gbps	-	-	-	-	-	-
Other	SAS2 Key Mobile Rack KVM Keyboard 17" LCD Monitor GigE switch 2x1.5 KW UPS's						External eSATA Dual Drive Bay w/ 3TB SATAII drive

PeDAL – The APDL Editor

- Side-by-side editor and help viewer layout.
- Instant help on any documented APDL command by pressing F1.
- Full syntax highlighting for ANSYS v12 Mechanical APDL.
- Auto-complete drop downs for APDL Commands.
- APDL Command argument hints while typing commands.
- Search ANSYS help phrases and keywords.
- Multiple tabs for the editor and html viewer.
- Full capability web browser built in allows for rich web experience and web searches.



Moisture Diffusion Modeling in MAPDL

Prepared by: Matt Sutton, PADT
With Input from Elana Antonova, ANSYS Inc

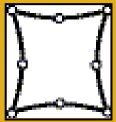
Coupled-Field Enhancements at 14.0

- New at 14.0
  - Diffusion physics and coupled-diffusion analyses
    - Thermal-diffusion
    - Structural-diffusion
    - Structural-thermal-diffusion
- Motivation
  - Simulation of moisture diffusion
  - Sodium migration in aluminum reduction cells

Elements for Coupled-Diffusion Analyses

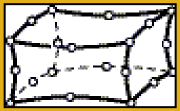
PLANE223

2-D 8-node quadrilateral



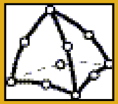
SOLID226

3-D 20-node brick



SOLID227

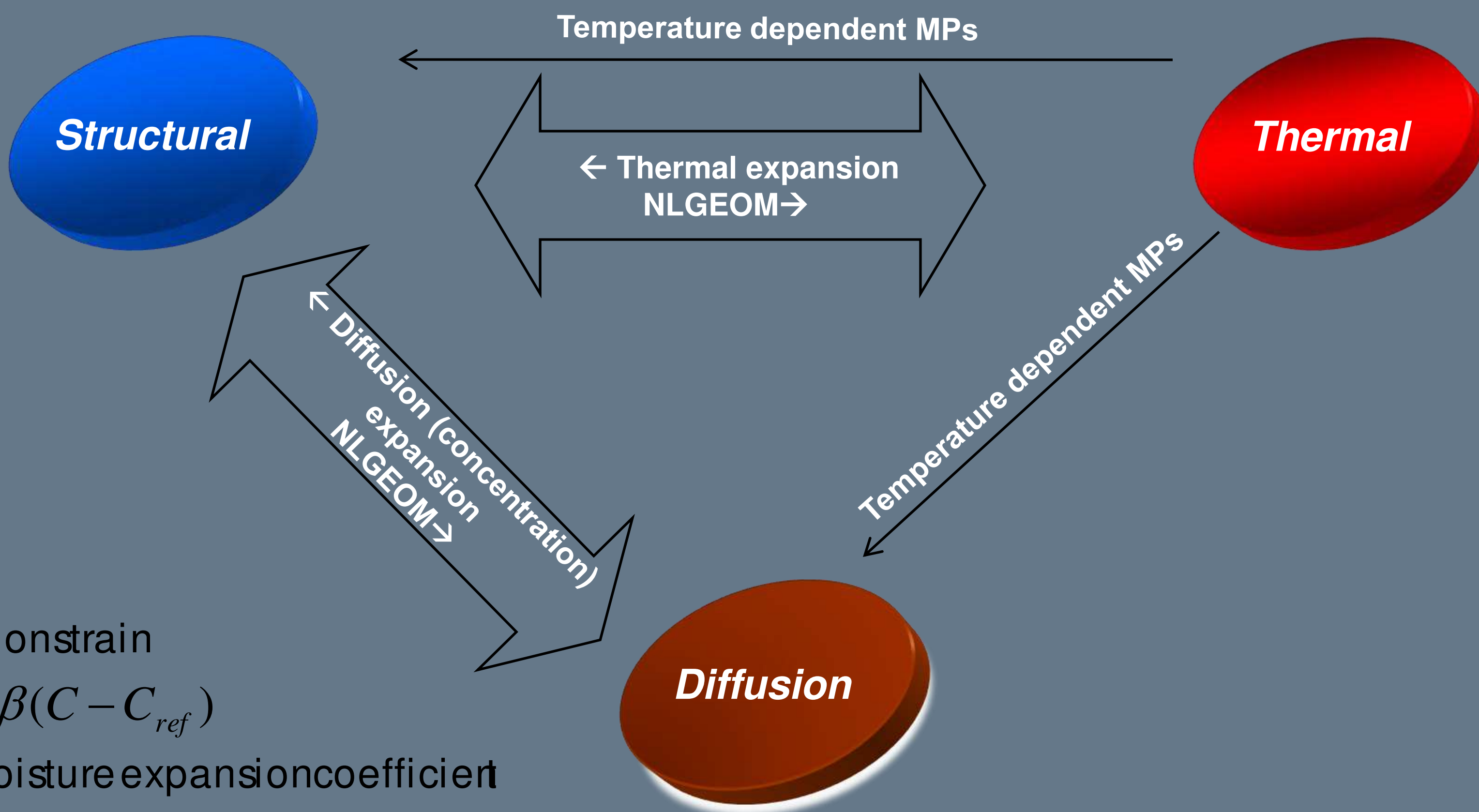
3-D 10-node tetrahedron



- KEYOPT(1) controls physics DoFs
  - KEYOPT(1)=100001 is structural-diffusion (U+CONC)
  - KEYOPT(1)=100010 is thermal-diffusion (TEMP+CONC)
  - KEYOPT(1)=100011 is structural-thermal-diffusion (U+TEMP+CONC)
- Material properties required
  - **MP**,DXX (DYY, DZZ) for diffusivity
  - **MP**,CSAT for saturated concentration
  - **MP**,BETX (BETY, BETZ) for coefficients of diffusion expansion
  - **MP**,CREF for reference concentration
  - All materials can be temperature-dependent
- Boundary conditions
  - **D**,,CONC and **IC**,,CONC for concentration
  - **F**,,RATE for diffusion flow rate
- Results
  - Concentration gradient (CG)
  - Diffusion flux (DF)
  - Diffusion strain (EPDI)

Coupled Effects in Structural-Thermal-Diffusion Analyses (14.0)

Thermal strain $\varepsilon^{th} = \alpha(T - T_{ref})$



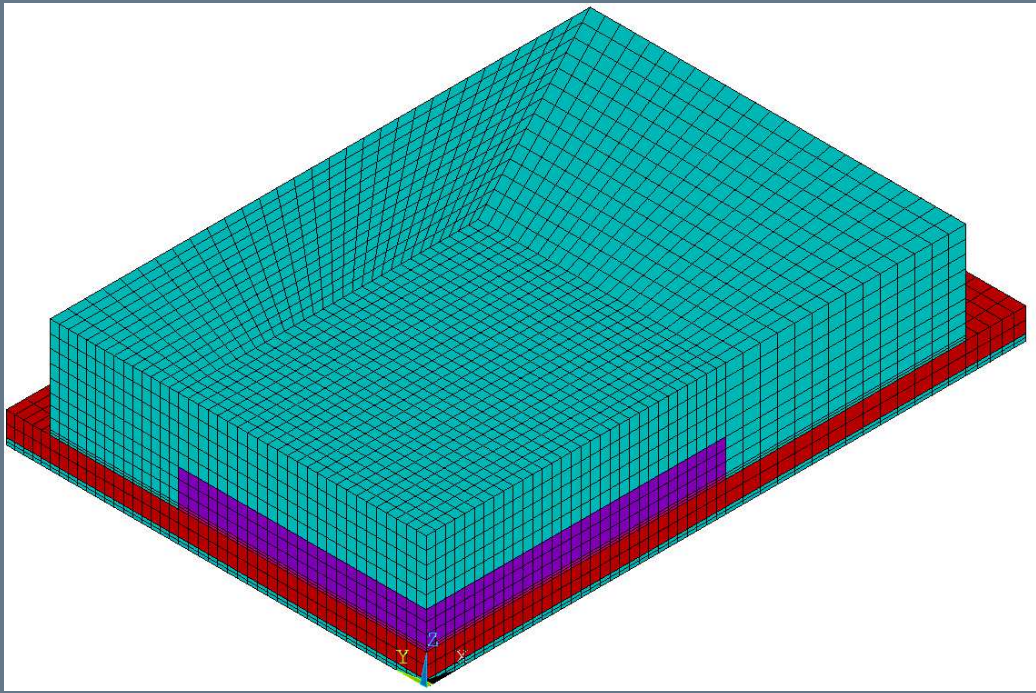
Diffusion strain

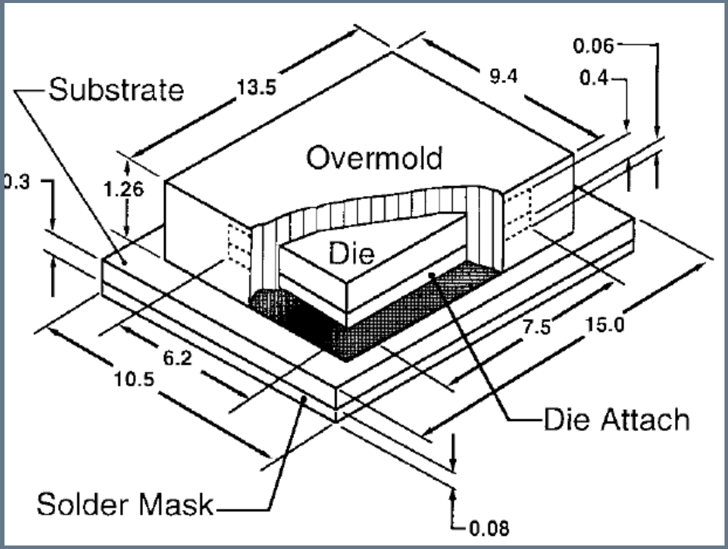
$\varepsilon^{di} = \beta(C - C_{ref})$

β - moisture expansion coefficient

C_{ref} - "reference" concentration

Example Model From Galloway and Miles.

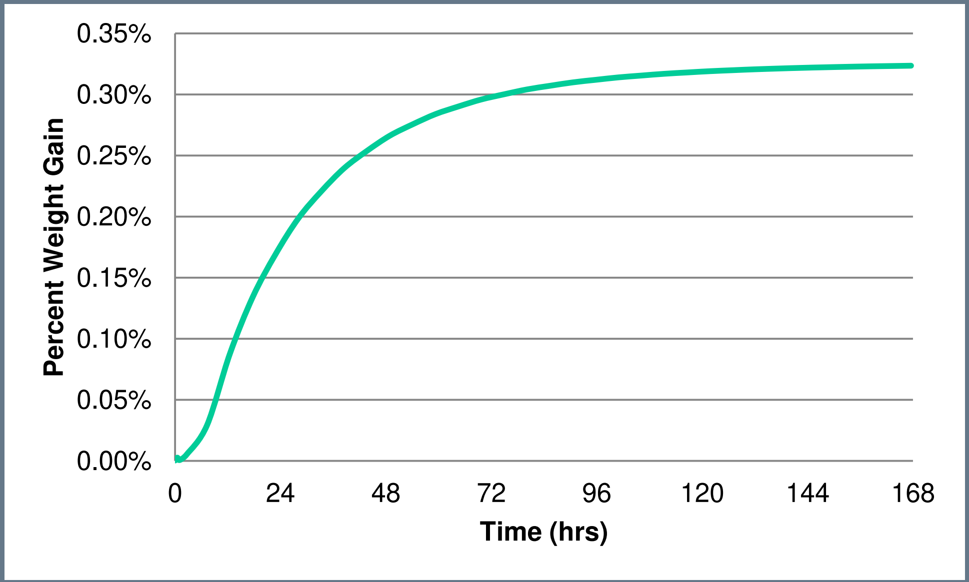


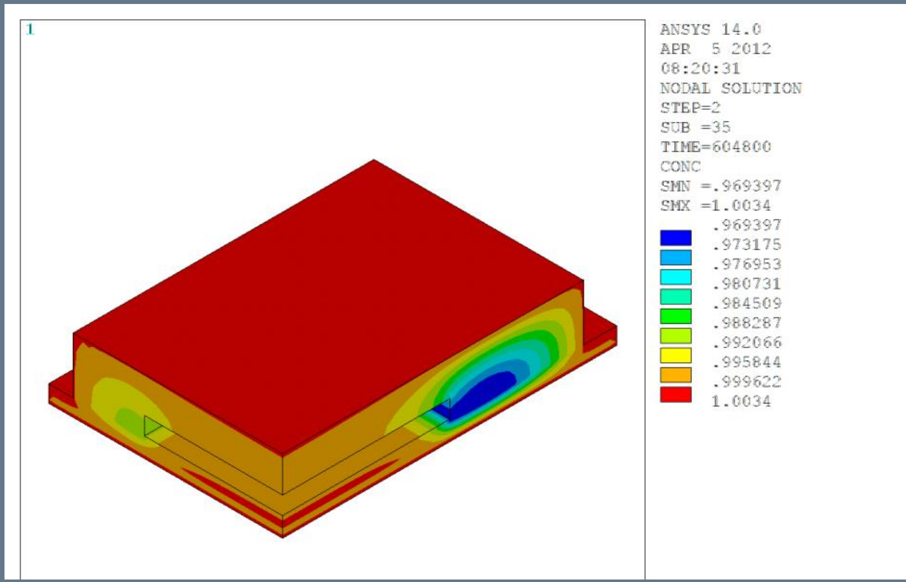


Geometry and ¼ Symmetry ANSYS Model

1. ANSYS model consists of solid226 with thermal and diffusion DOFS
2. Die is modeled with solid70s (thermal only)
3. Material properties are temp dependent

Results for 85C/85% RH for 168 Hours





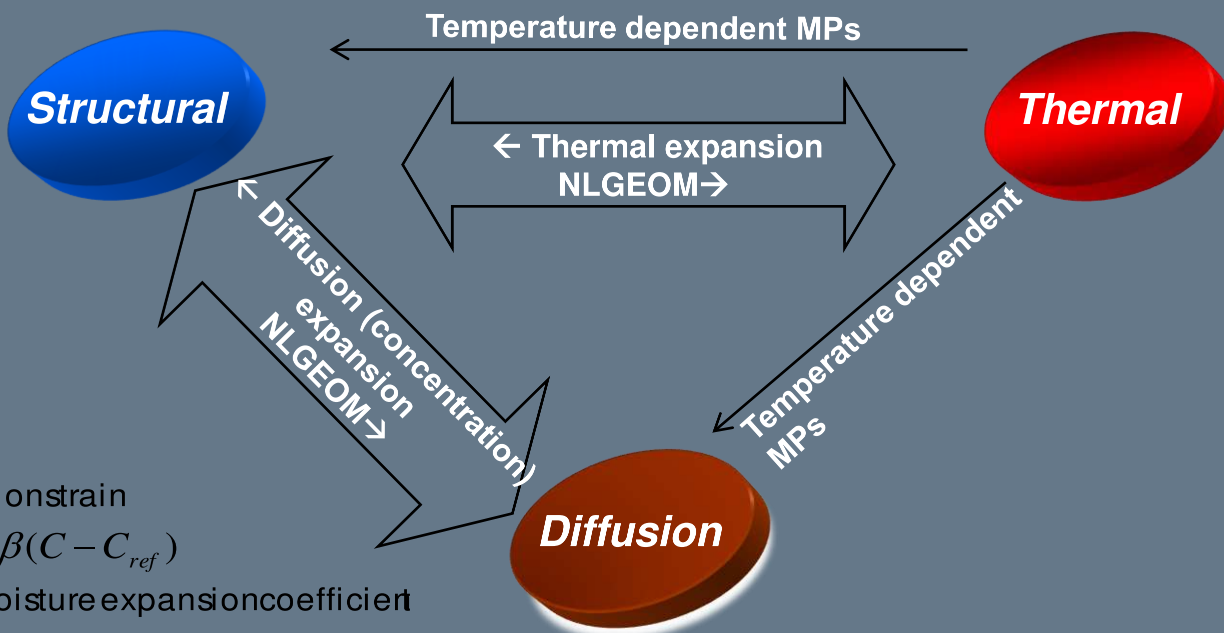
Model is run as a transient, but since the temperature is constant and the thermal time scale is much smaller than the diffusion time scale, you can turn thermal time integration off.

Post process to get percent weight gain as a function of time.

“Popcorn” Modeling

- Use cohesive zone elements to model delamination
- Use Solid226 to model thermal/structural/diffusion interaction

Thermal strain $\varepsilon^{th} = \alpha(T - T_{ref})$



Diffusion strain

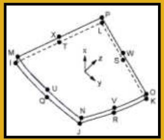
$\varepsilon^{di} = \beta(C - C_{ref})$

β - moisture expansion coefficient

C_{ref} - "reference" concentration

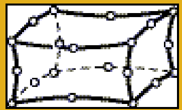
INTER204

3-D 16-node interface



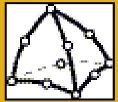
SOLID226

3-D 20-node Brick



SOLID227

3-D 10-node tetrahedron

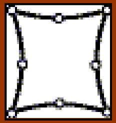


Diffusion Analysis at 14.5

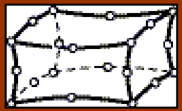
- New at 14.5
  - Three high-order elements for a standard diffusion analysis
    - PLANE238 – 2D 8-node quadrilateral
    - SOLID239 – 3D 20-node hexahedral
    - SOLID240 – 3D 10-node tetrahedron
- Motivation
  - Prior to 14.0, a temperature-concentration analogy was used to model diffusion
    - Valid only for homogeneous materials
  - For inhomogeneous materials, a *normalized concentration* approach is available with the new elements
    - Unlike temperature, concentration is *discontinuous* across material interfaces since it is limited by saturated concentration, which is different for different materials. Normalized concentration $\varphi = C/C_{sat}$ is continuous across material interfaces, so this is the DoF used in moisture diffusion problems.

New Elements for Diffusion Analysis

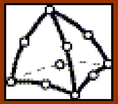
<u>PLANE238</u>
2-D 8-node quadrilateral



<u>SOLID239</u>
3-D 20-node brick



<u>SOLID240</u>
3-D 10-node tetrahedron



- Degrees of freedom
  - CONC – concentration or normalized concentration (if Csat specified)
- Material properties (**MP**)
  - DXX, DYY, DZZ, CSAT
- Surface loads (**SF**)
  - Diffusion flux (DFLUX)
- Body loads (**BF**)
  - Diffusing substance generation rate (DGEN)
- Boundary conditions
  - **D**,,CONC and **IC**,,CONC for concentration
  - **F**,,RATE for diffusion flow rate
- Results
  - Concentration gradient (CG)
  - Diffusion flux (DF)

Will be supported by the 22x elements

Coupled-Field Enhancements at 14.5/15.0 (Subject to Change)

- Current development
  - Support structural material nonlinearities (plasticity, viscoelasticity)
  - Couple diffusion with electric and electrostatic fields
    - Structural-thermo-electric-diffusion analysis
    - Electrostatic-diffusion analysis
- Motivation
  - Enhance moisture migration analysis
  - Electromigration in solder joints

Driving Forces of Electromigration

- Atomic concentration
- Thermal gradient
- Electric field
- Stress gradient

Mass conservation $\nabla \cdot \vec{J} + \frac{\partial c}{\partial t} = 0$

Atomic flux $\vec{J} = -D\left(\nabla c + \frac{cQ^*}{kT^2} \nabla T + \frac{cZ^* e}{kT} \nabla \varphi + \frac{c\Omega}{kT} \nabla \sigma \right)$

Q^* - heat of transport

Z^* - effective charge

Ω - atomic volume

More Coupled Diffusion Analyses in 15.0 (Subject to Change)