# *Advanced Gas Reactor Fuels Program Review*

# *AGR-2 Safety Test Predictions Using PARFUME*

**Blaise Collin**
**Irradiations & Fuel Performance Modeling**

**July 15-16, 2015**

www.inl.gov

Idaho National Laboratory

# *Compact selection*

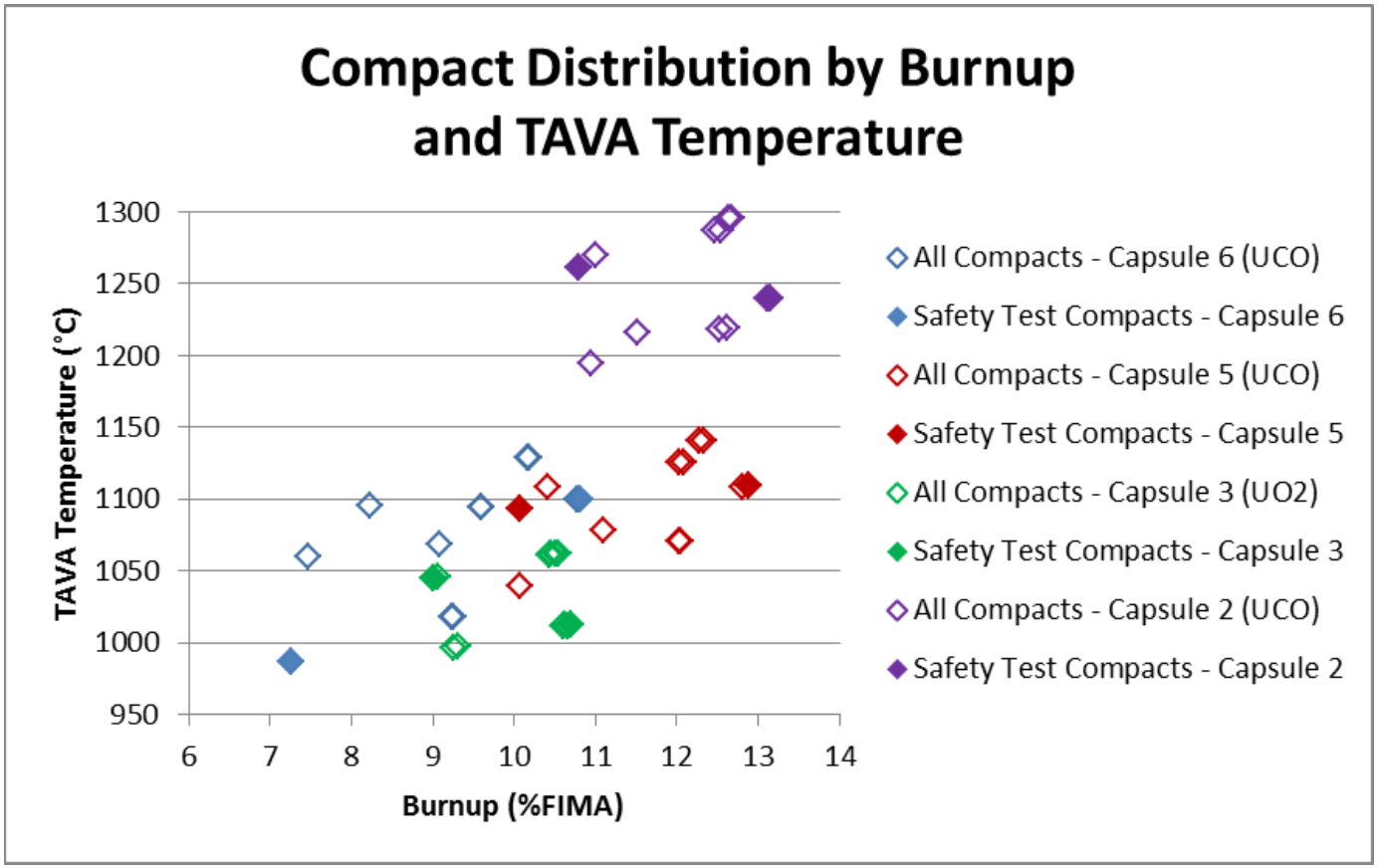
**Two Compacts per Capsule:** min & max BU/FF

**2-2-3 (10.80/2.99)**
**2-4-2 (13.15/3.47)**

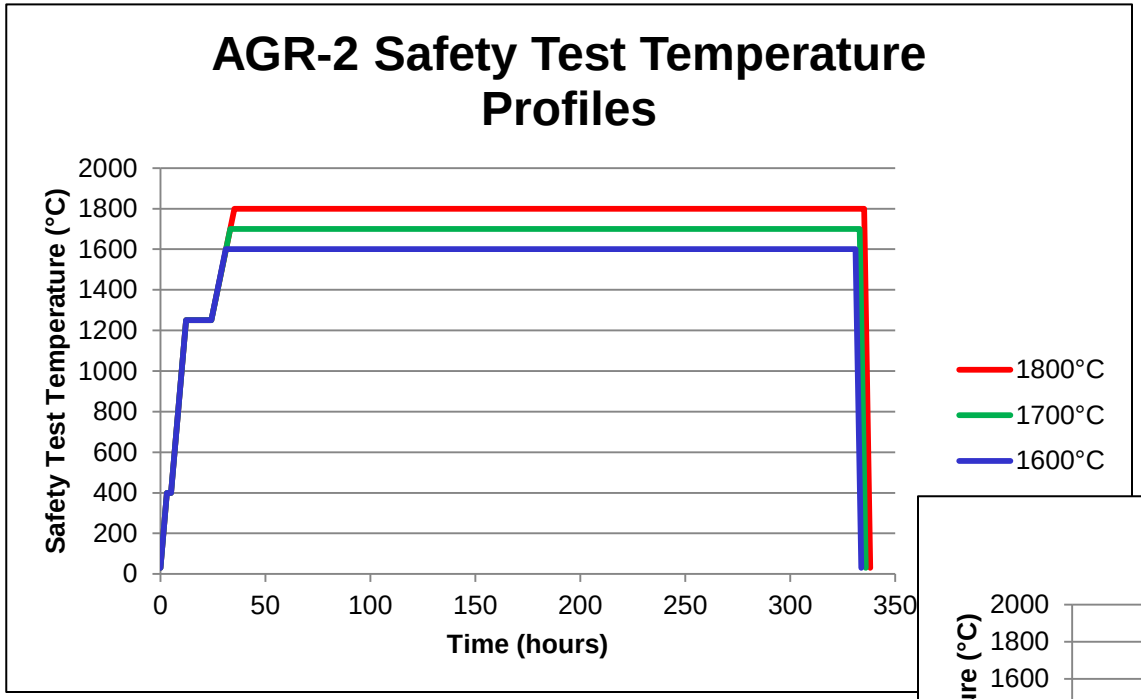
**3-2-3 (9.01/3.09)**
**3-4-2 (10.69/3.50)**

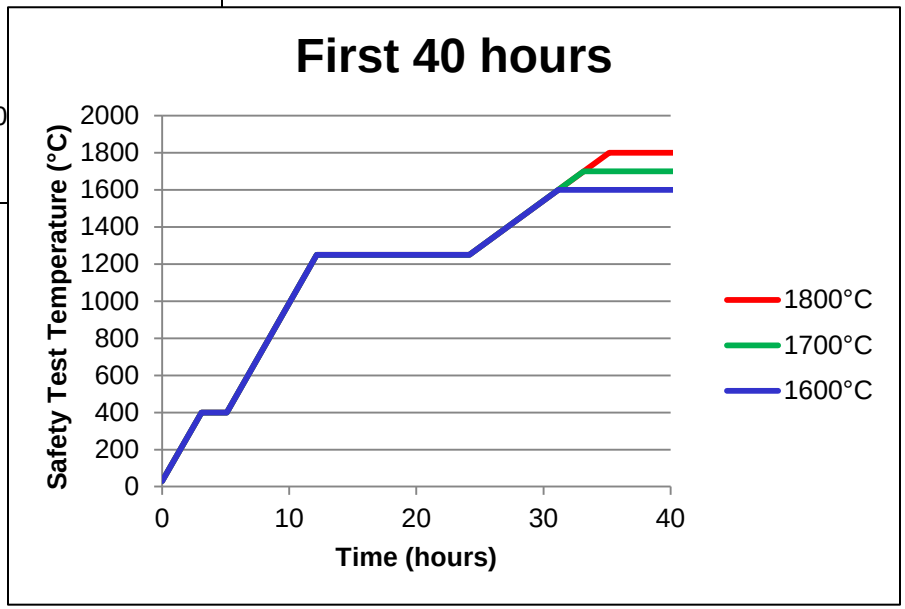
**5-1-2 (12.88/3.42)**
**5-3-3 (10.07/2.91)**

**6-1-2 (10.81/2.73)**
**6-4-3 (7.26/1.94)**



# *Safety Test – Temperature Profiles*




**300-hour heat-up at**
**1600, 1700, and 1800°C**

# *PARFUME Calculations*

- Failure probability
  - IPyC cracking (→ SiC failure)
  - Pressure (→ (full) particle failure)

- Palladium penetration

- Fission product release
  - Ag, Cs, Sr, Kr

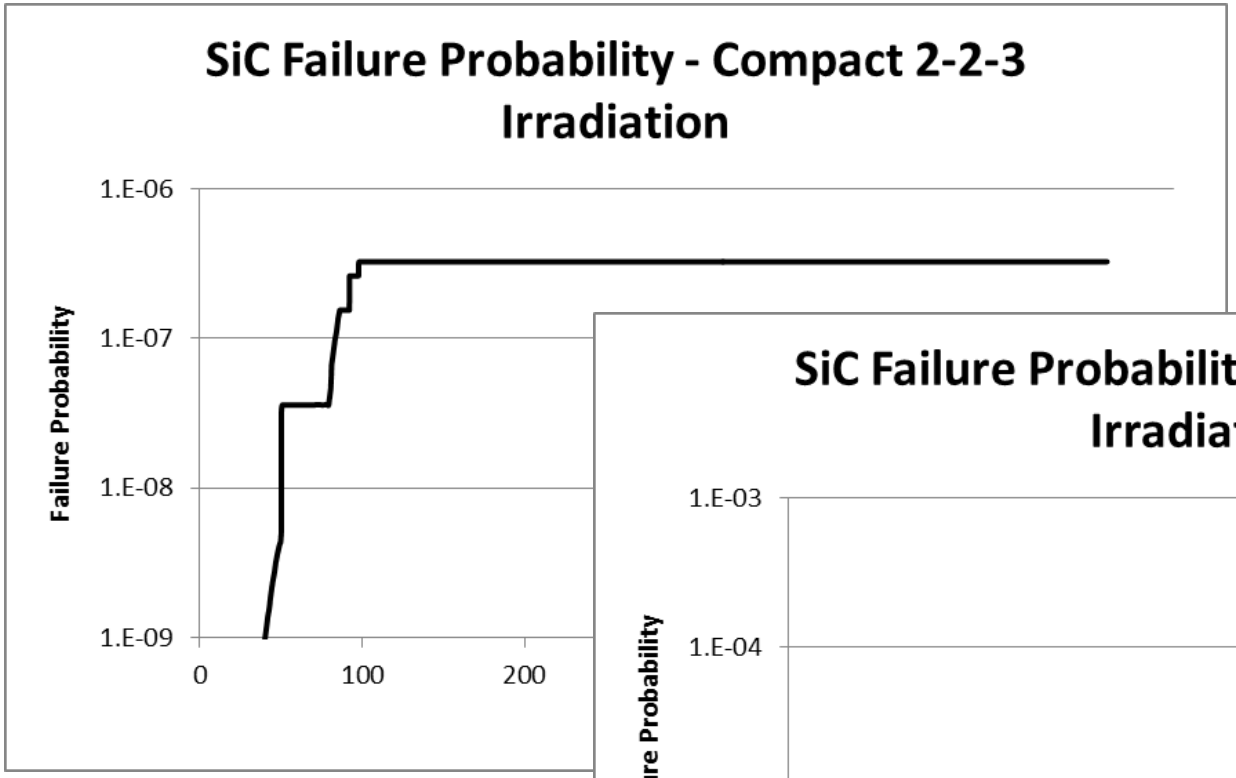
→ includes end-of-irradiation and safety testing results
→ includes intact particles and 1 particle with initially exposed kernel

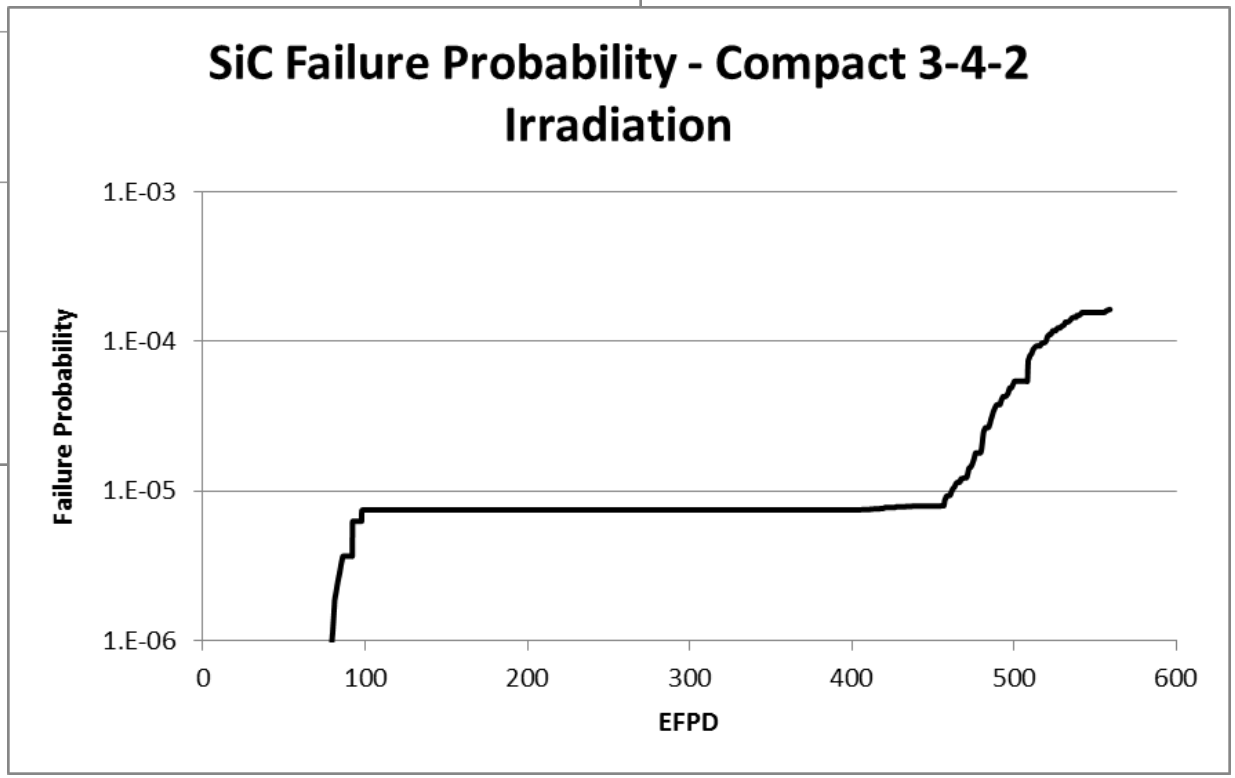
- No particle failure observed during irradiation
- 0-1 ($UO_2$) and 2-3 (UCO) initially exposed kernels per capsule (cf. monitoring of fission gas release)

# Failure Probability – Irradiation

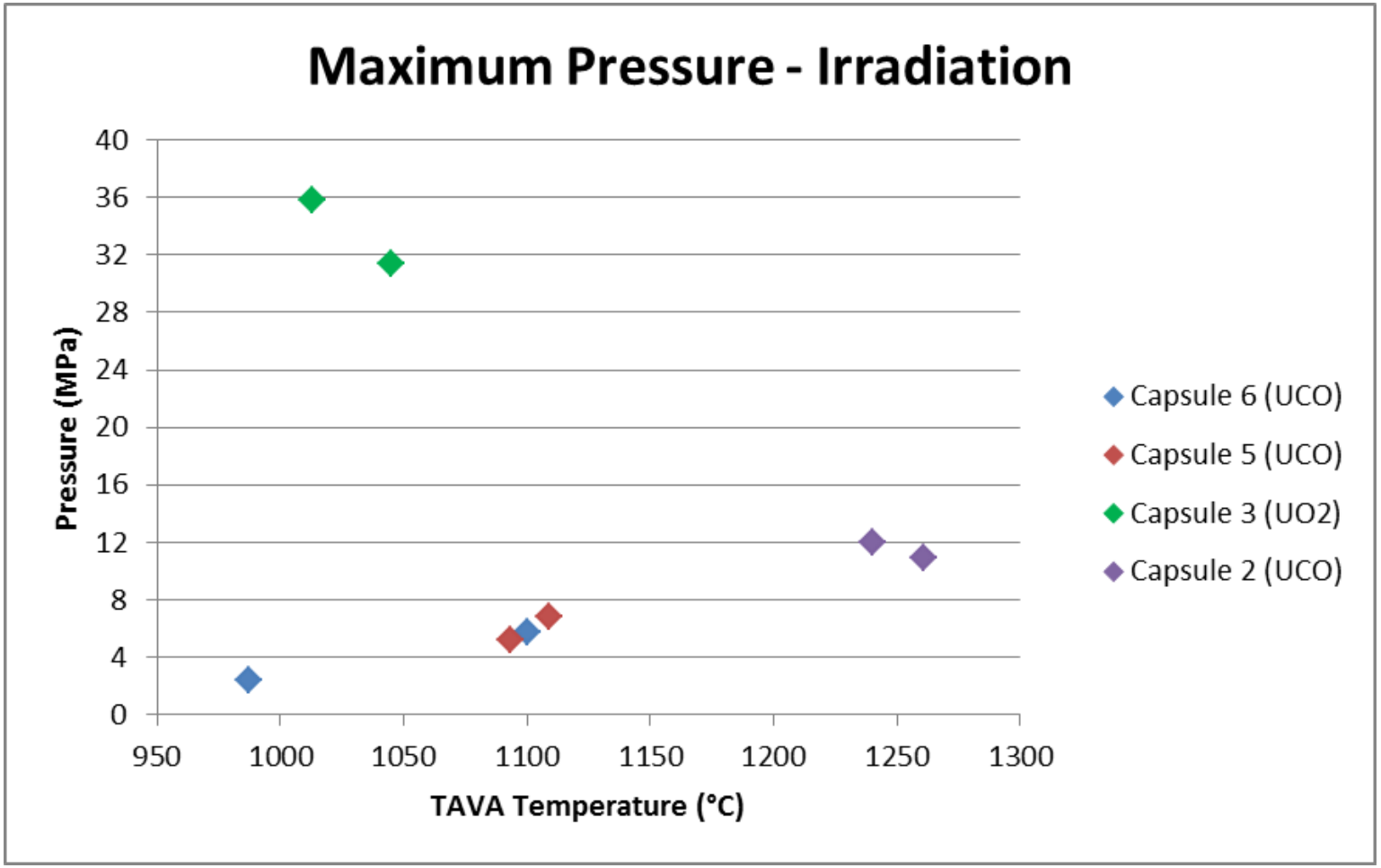
| Compact | Fuel | Probability of SiC failure | | | Probability of IPyC Cracking | Number of Failed Particles |
|---|---|---|---|---|---|---|
| | | Total | IPyC Cracking | Pressure | | |
| 6-4-3 | UCO | $3.5\times10^{-5}$ | $3.5\times10^{-5}$ | 0 | $3.1\times10^{-1}$ | 0 |
| 6-1-2 | | $3.0\times10^{-6}$ | $3.0\times10^{-6}$ | 0 | $7.9\times10^{-2}$ | 0 |
| 5-3-3 | UCO | $5.5\times10^{-6}$ | $5.5\times10^{-6}$ | 0 | $1.2\times10^{-1}$ | 0 |
| 5-1-2 | | $2.1\times10^{-6}$ | $2.1\times10^{-6}$ | 0 | $5.1\times10^{-2}$ | 0 |
| 3-4-2 | $UO_2$ | $1.6\times10^{-4}$ | $7.5\times10^{-6}$ | $1.6\times10^{-4}$ | $1.6\times10^{-1}$ | 0 |
| 3-2-3 | | $2.2\times10^{-5}$ | $9.1\times10^{-6}$ | $1.3\times10^{-5}$ | $1.7\times10^{-1}$ | 0 |
| 2-4-2 | UCO | $7.5\times10^{-8}$ | $7.5\times10^{-8}$ | 0 | $1.2\times10^{-2}$ | 0 |
| 2-2-3 | | $3.3\times10^{-7}$ | $3.3\times10^{-7}$ | 0 | $2.9\times10^{-2}$ | 0 |

# Failure Probability – Irradiation



# Failure Probability – Irradiation



# Failure Probability – Irradiation + ST (1600°C)

| Compact | Fuel | Probability of SiC failure | | | Probability of IPyC Cracking | Number of Failed Particles |
|---|---|---|---|---|---|---|
| | | Total | IPyC Cracking | Pressure | | |
| 6-4-3 | UCO | $3.5\times10^{-5}$ | $3.5\times10^{-5}$ | 0 | $3.1\times10^{-1}$ | 0 |
| 6-1-2 | | $3.0\times10^{-6}$ | $3.0\times10^{-6}$ | 0 | $7.9\times10^{-2}$ | 0 |
| 5-3-3 | UCO | $5.5\times10^{-6}$ | $5.5\times10^{-6}$ | 0 | $1.2\times10^{-1}$ | 0 |
| 5-1-2 | | $2.1\times10^{-6}$ | $2.1\times10^{-6}$ | 0 | $5.1\times10^{-2}$ | 0 |
| 3-4-2 | $UO_2$ | $1.3\times10^{-2}$ | $7.5\times10^{-6}$ | $1.3\times10^{-2}$ | $1.6\times10^{-1}$ | 20 |
| 3-2-3 | | $1.6\times10^{-3}$ | $9.1\times10^{-6}$ | $1.6\times10^{-3}$ | $1.7\times10^{-1}$ | 2 |
| 2-4-2 | UCO | $7.5\times10^{-8}$ | $7.5\times10^{-8}$ | $2.3\times10^{-11}$ | $1.3\times10^{-2}$ | 0 |
| 2-2-3 | | $3.3\times10^{-7}$ | $3.3\times10^{-7}$ | $4.3\times10^{-17}$ | $2.9\times10^{-2}$ | 0 |

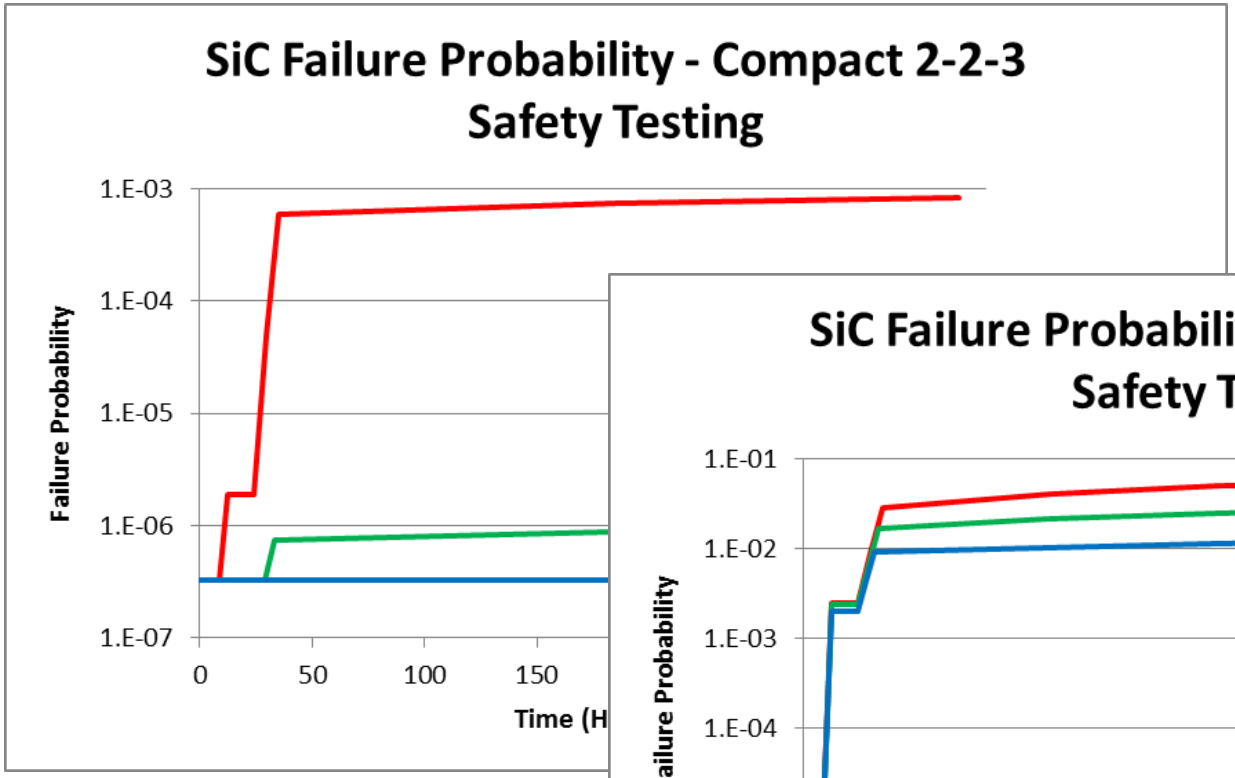
# Failure Probability – Irradiation + ST (1700°C)

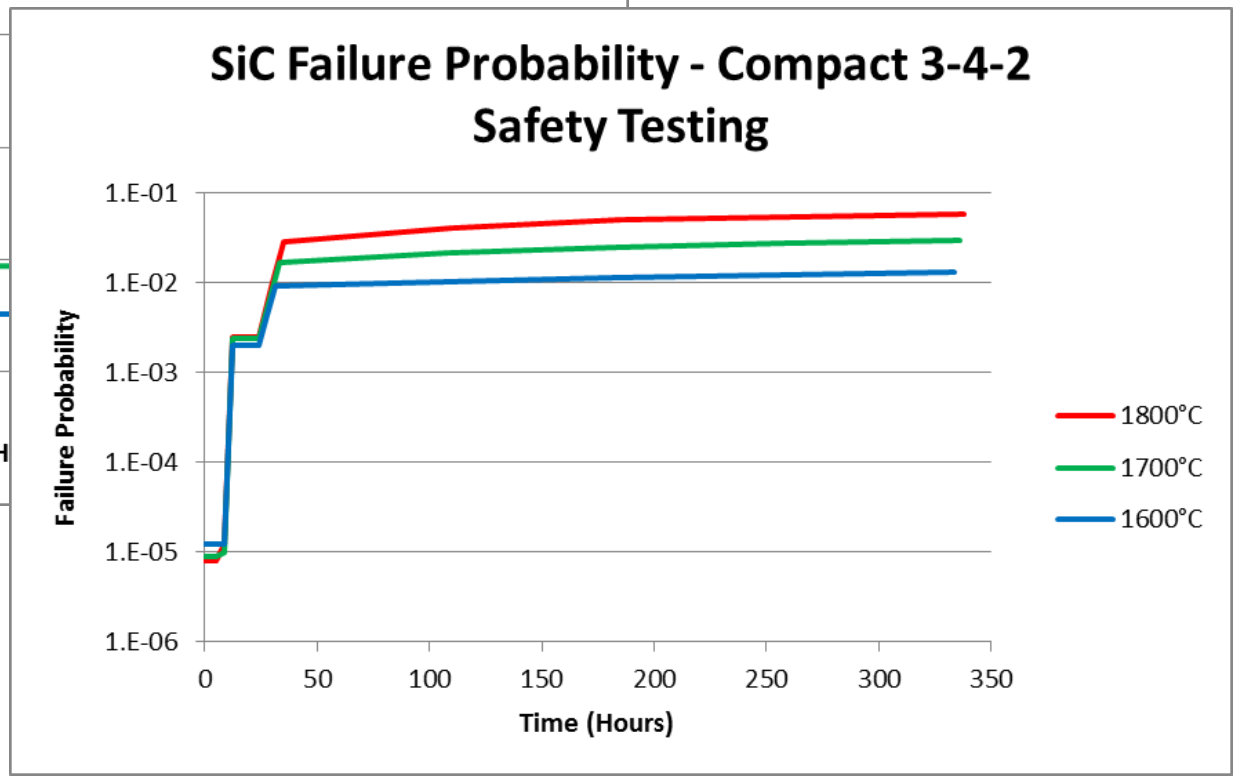
| Compact | Fuel | Probability of SiC failure | | | Probability of IPyC Cracking | Number of Failed Particles |
|---|---|---|---|---|---|---|
| | | Total | IPyC Cracking | Pressure | | |
| 6-4-3 | UCO | $3.5\times10^{-5}$ | $3.5\times10^{-5}$ | 0 | $3.1\times10^{-1}$ | 0 |
| 6-1-2 | | $3.0\times10^{-6}$ | $3.0\times10^{-6}$ | 0 | $7.9\times10^{-2}$ | 0 |
| 5-3-3 | UCO | $5.5\times10^{-6}$ | $5.5\times10^{-6}$ | 0 | $1.2\times10^{-1}$ | 0 |
| 5-1-2 | | $2.3\times10^{-6}$ | $2.1\times10^{-6}$ | $1.3\times10^{-7}$ | $5.1\times10^{-2}$ | 0 |
| 3-4-2 | $UO_2$ | $3.0\times10^{-2}$ | $7.5\times10^{-6}$ | $3.0\times10^{-2}$ | $1.6\times10^{-1}$ | 46 |
| 3-2-3 | | $4.1\times10^{-3}$ | $9.1\times10^{-6}$ | $4.1\times10^{-3}$ | $1.7\times10^{-1}$ | 6 |
| 2-4-2 | UCO | $3.3\times10^{-5}$ | $7.5\times10^{-8}$ | $3.2\times10^{-5}$ | $1.2\times10^{-2}$ | 0 |
| 2-2-3 | | $1.0\times10^{-6}$ | $3.3\times10^{-7}$ | $7.0\times10^{-7}$ | $2.9\times10^{-2}$ | 0 |

# Failure Probability – Irradiation + ST (1800°C)

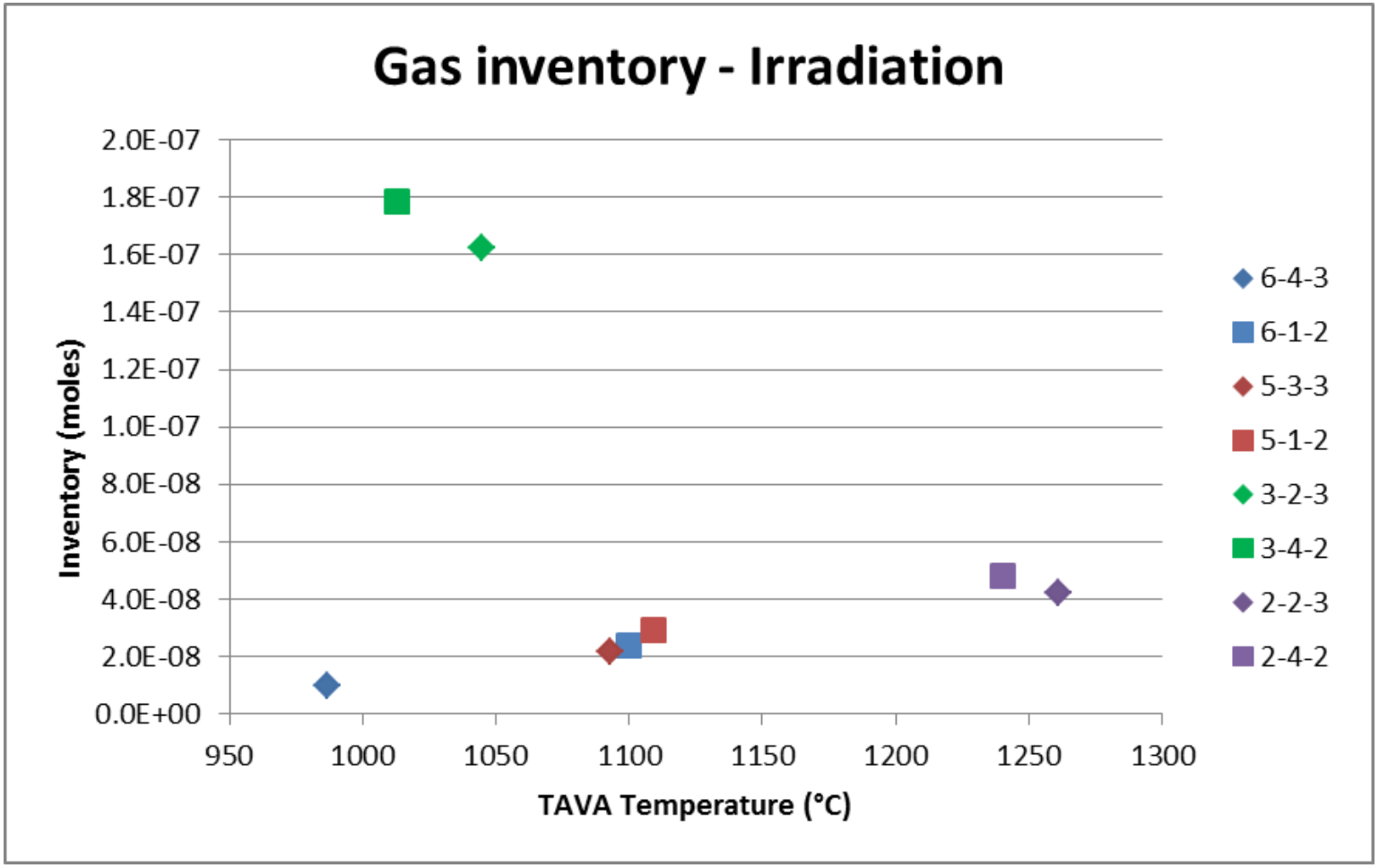
| Compact | Fuel | Probability of SiC failure | | | Probability of IPyC Cracking | Number of Failed Particles |
|---|---|---|---|---|---|---|
| | | Total | IPyC Cracking | Pressure | | |
| 6-4-3 | UCO | $3.5\times10^{-5}$ | $3.5\times10^{-5}$ | 0 | $3.1\times10^{-1}$ | 0 |
| 6-1-2 | | $8.4\times10^{-6}$ | $3.0\times10^{-6}$ | $5.5\times10^{-6}$ | $7.9\times10^{-2}$ | 0 |
| 5-3-3 | UCO | $3.2\times10^{-5}$ | $5.5\times10^{-6}$ | $2.7\times10^{-5}$ | $1.2\times10^{-1}$ | 0 |
| 5-1-2 | | $1.4\times10^{-3}$ | $2.1\times10^{-6}$ | $1.4\times10^{-3}$ | $5.1\times10^{-2}$ | 4 |
| 3-4-2 | $UO_2$ | $5.8\times10^{-2}$ | $7.5\times10^{-6}$ | $5.8\times10^{-2}$ | $1.6\times10^{-1}$ | 90 |
| 3-2-3 | | $8.7\times10^{-3}$ | $9.1\times10^{-6}$ | $8.7\times10^{-3}$ | $1.7\times10^{-1}$ | 13 |
| 2-4-2 | UCO | $5.0\times10^{-3}$ | $7.5\times10^{-8}$ | $5.0\times10^{-3}$ | $1.2\times10^{-2}$ | 16 |
| 2-2-3 | | $8.4\times10^{-4}$ | $3.3\times10^{-7}$ | $8.4\times10^{-4}$ | $2.9\times10^{-2}$ | 3 |

# Failure Probability – Irradiation + ST

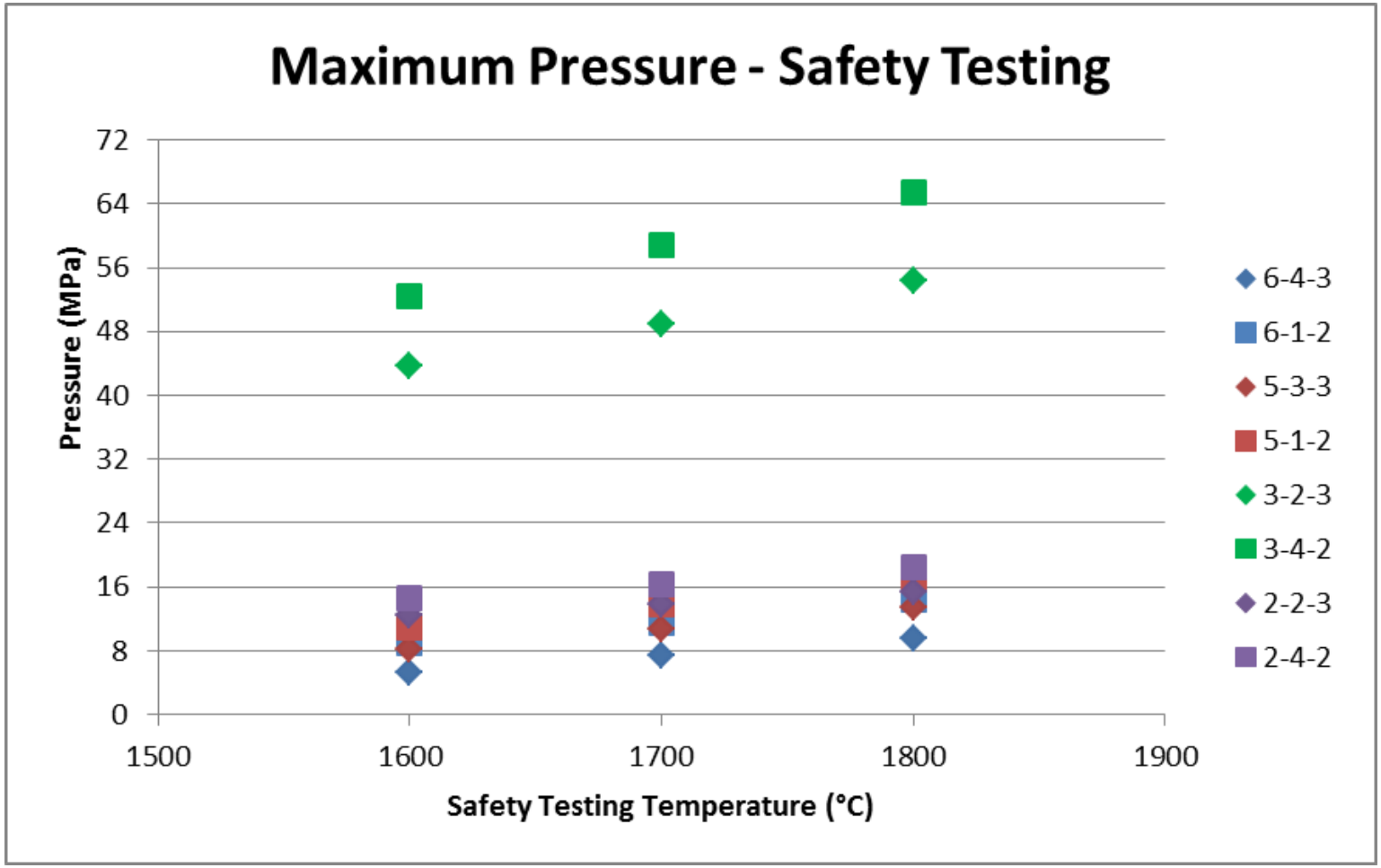


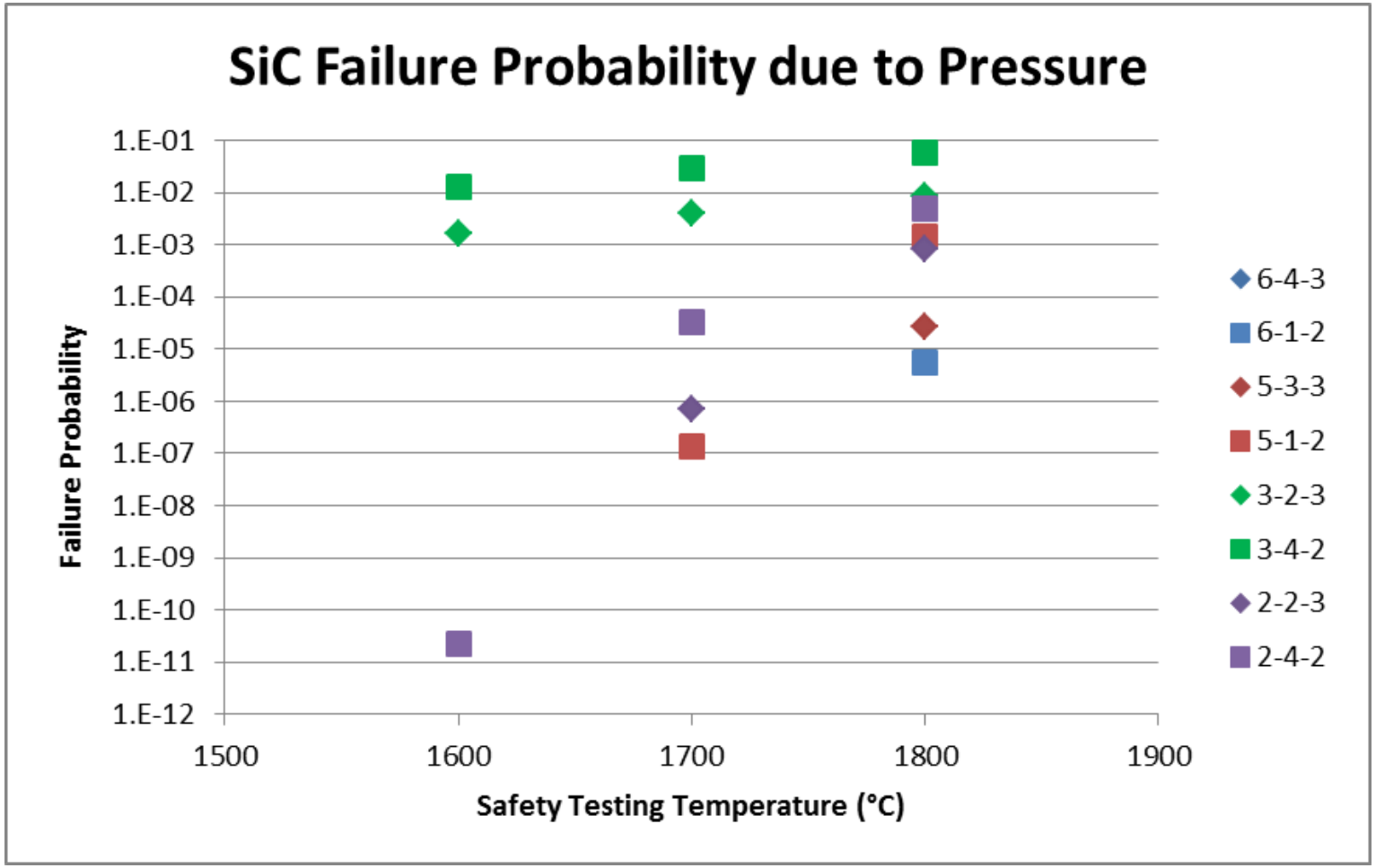
# Failure Probability – Irradiation + ST



# Failure Probability – Irradiation + ST



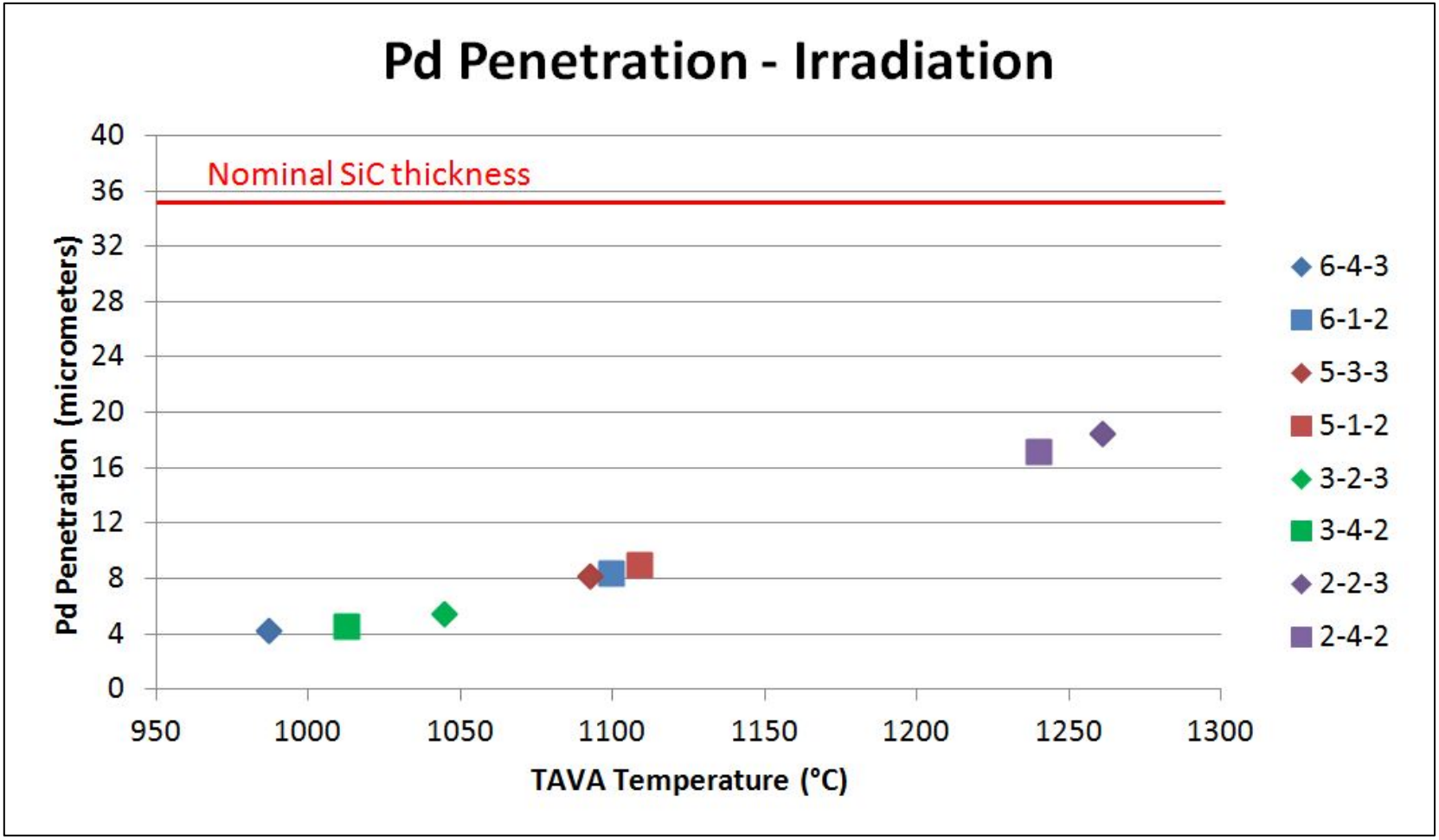
# Failure Probability – Irradiation + ST



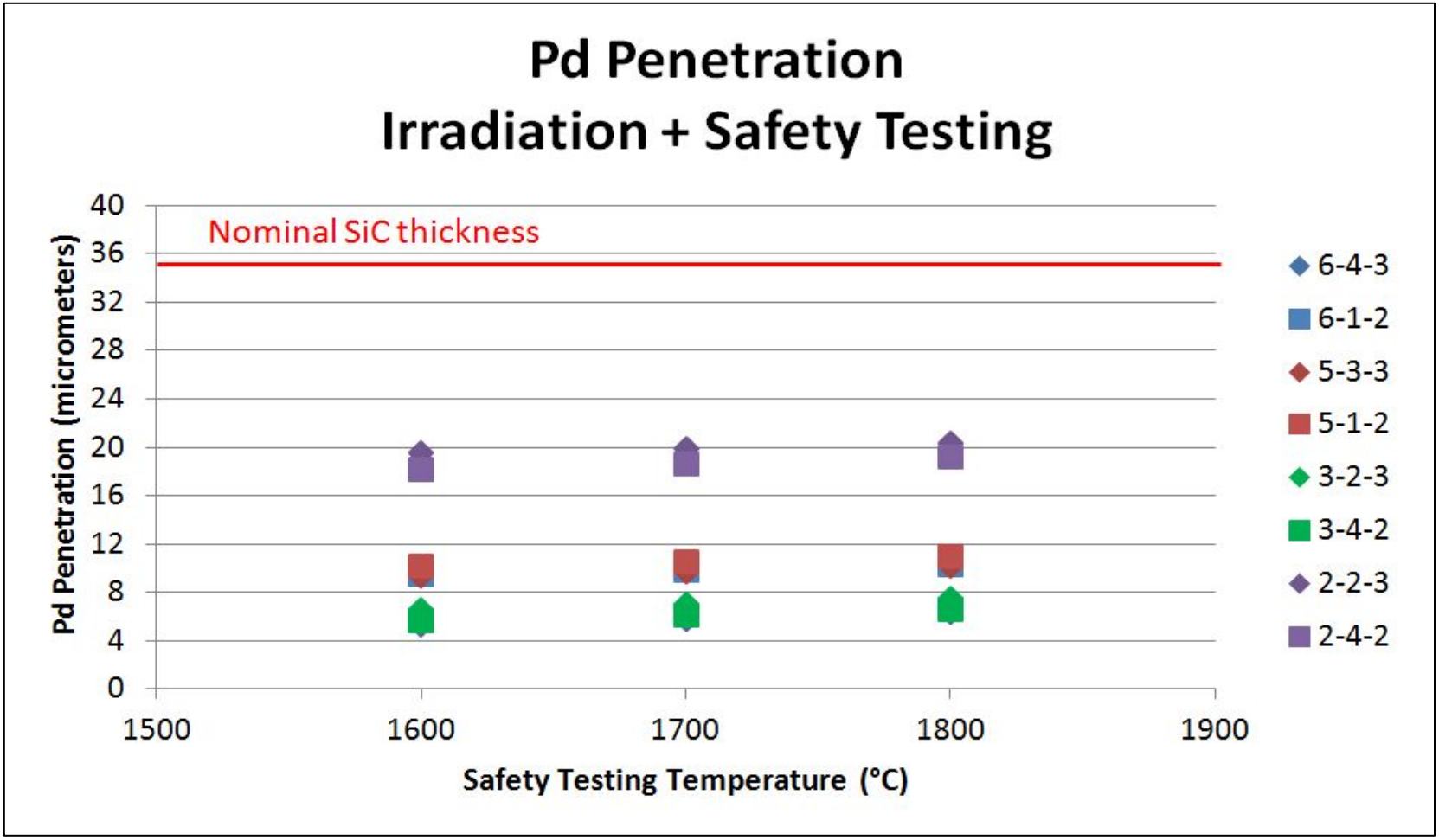
# *Failure Probability – Summary*

- No particle failure predicted during irradiation
- $UO_2$ → full failure at all ST temperatures (CO production)
- UCO → full failure at 1800°C (fission gases)
- No IPyC cracking during ST
- No failures predicted for AGR-1 (lower kernel temperature)
- Will PIE observe the predicted full failures during ST?

# Palladium Penetration - Irradiation



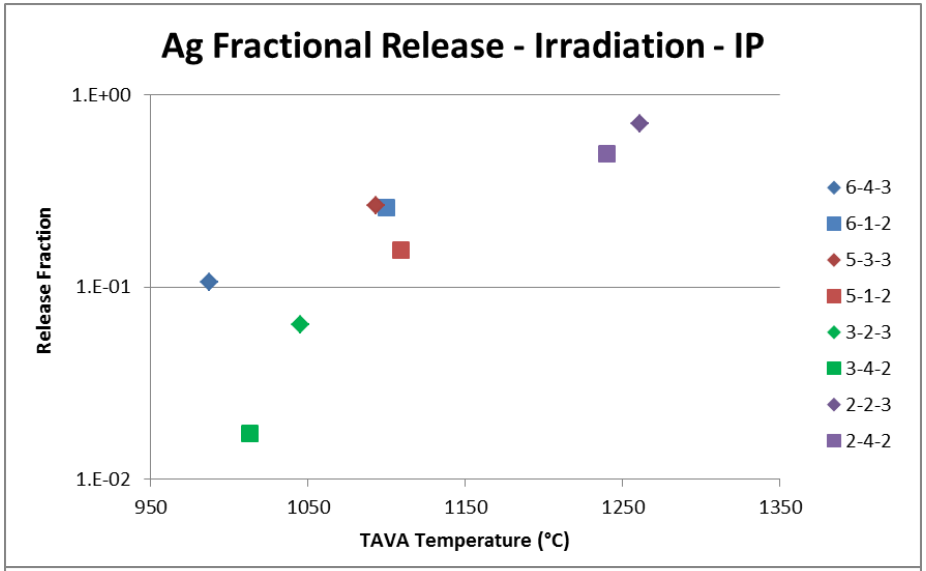
# Palladium Penetration – Irradiation + ST

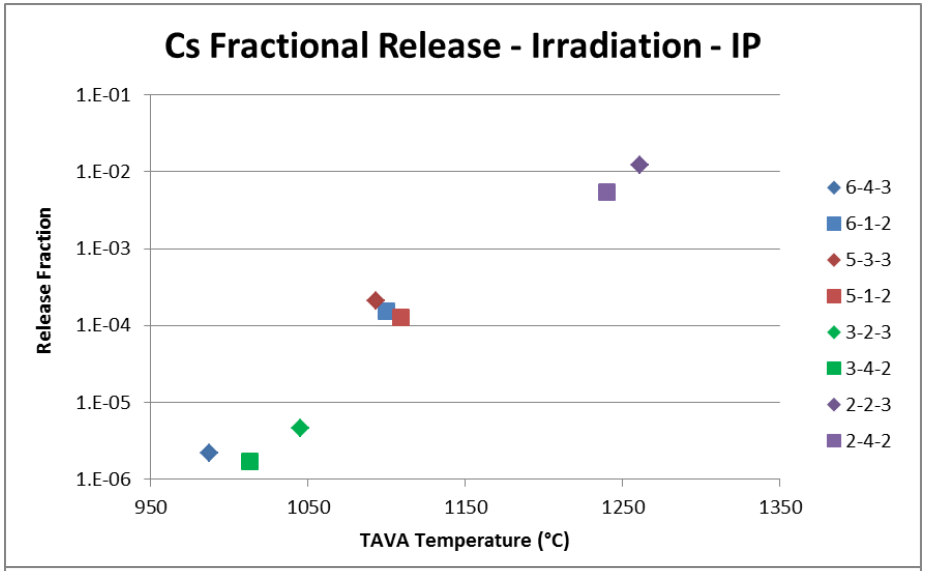


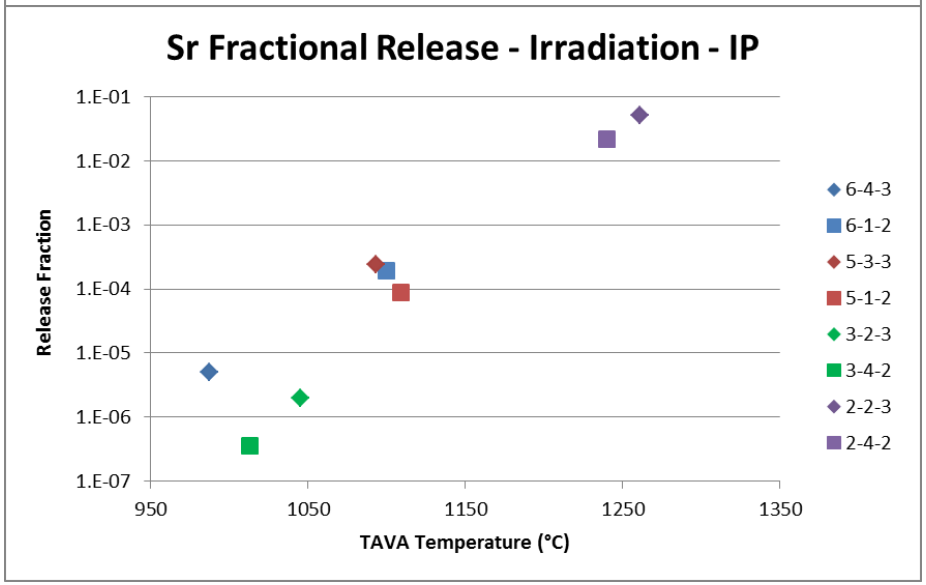
# *Fractional Release*

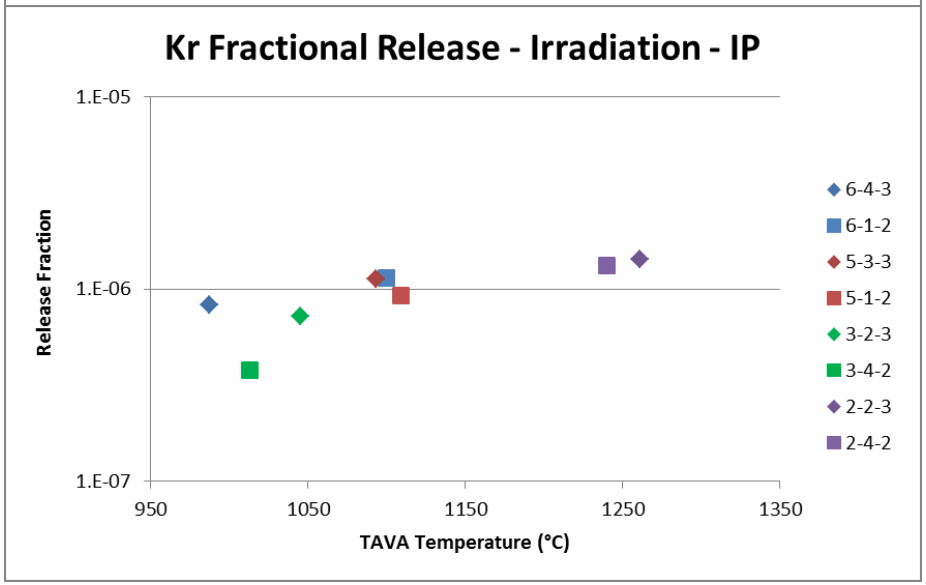
- No particle failure observed during irradiation
- Gas monitoring → 0-1 exposed kernel per $UO_2$ capsule
  2-3 exposed kernels per UCO capsule
- Irradiation: modeling of release from intact particle (IP) and exposed kernel (EK) separately and results combined to obtain release from compact ($UO_2$ 1543 p/c – UCO 3176 p/c)
- Release level of 1 particle: $UO_2$ $6.5\times10^{-4}$ – UCO $3.1\times10^{-4}$
- Safety Testing: intact particles during irradiation have a probability of SiC failure during ST due to pressure

# Fractional Release – Irradiation (IP)

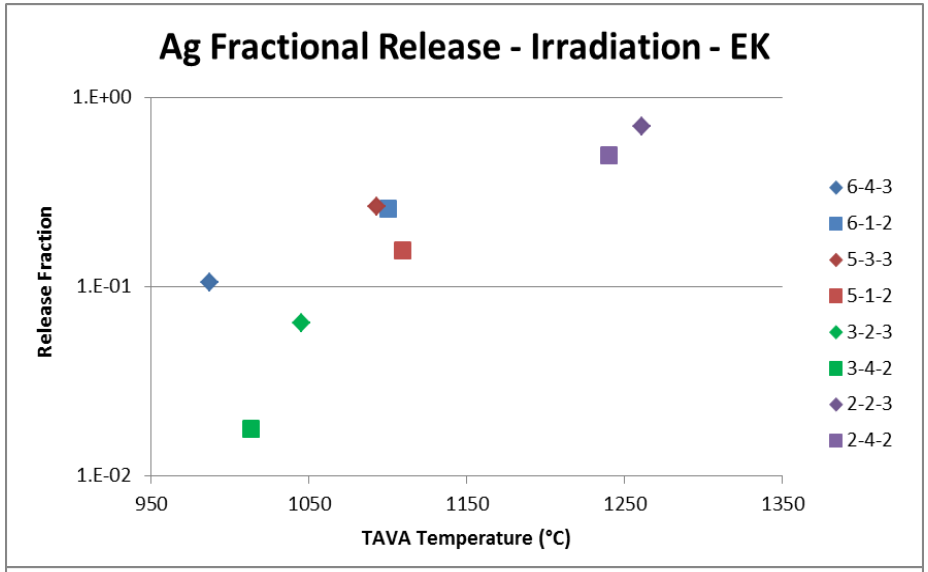


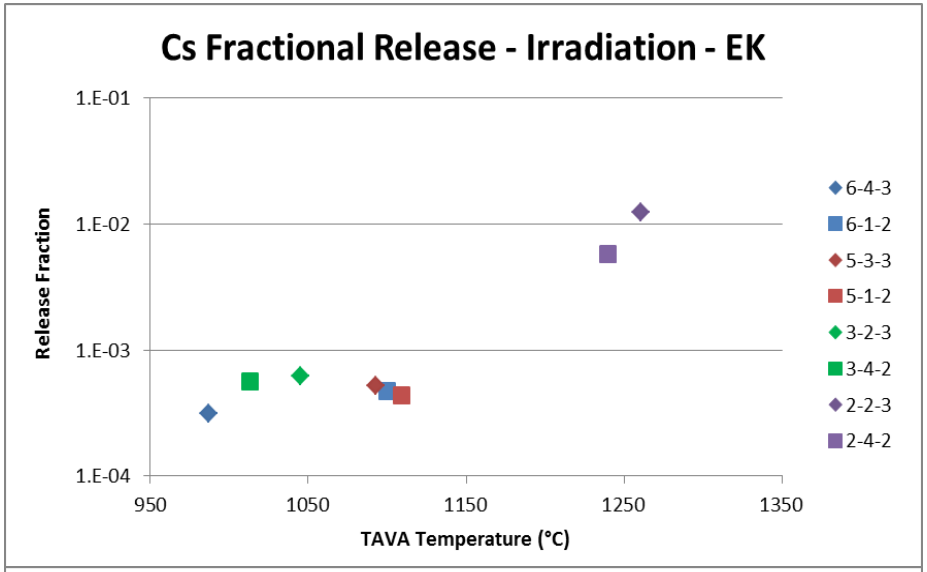



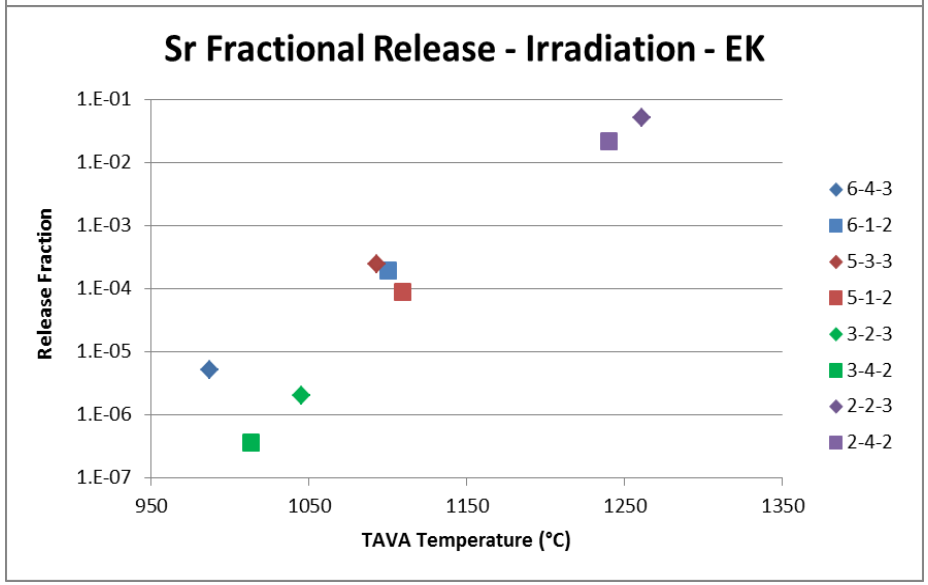



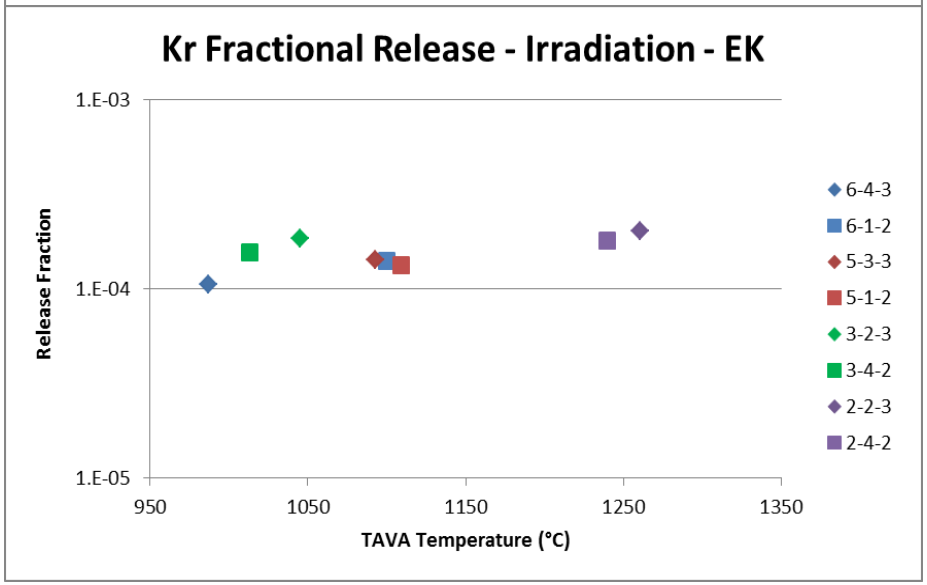



# Fractional Release – Irradiation (EK)

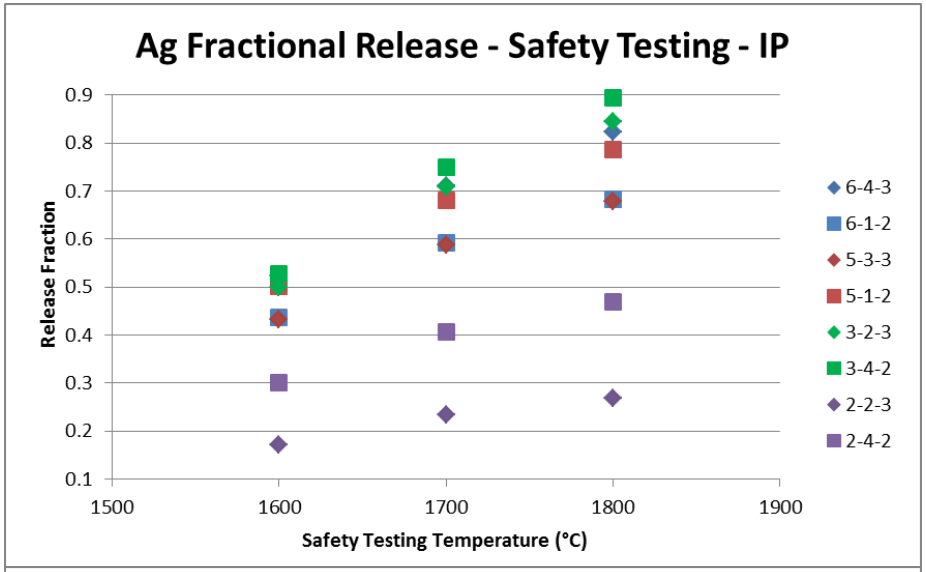


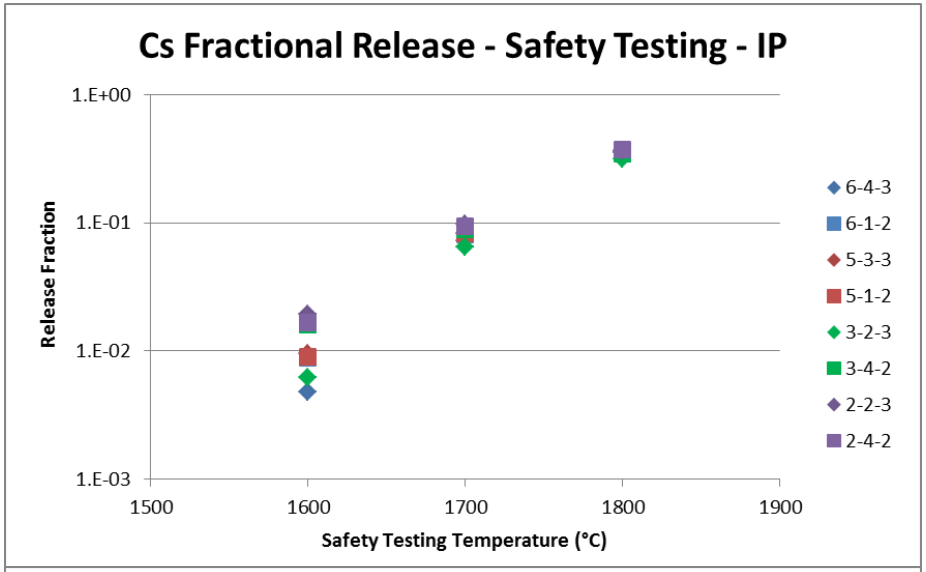



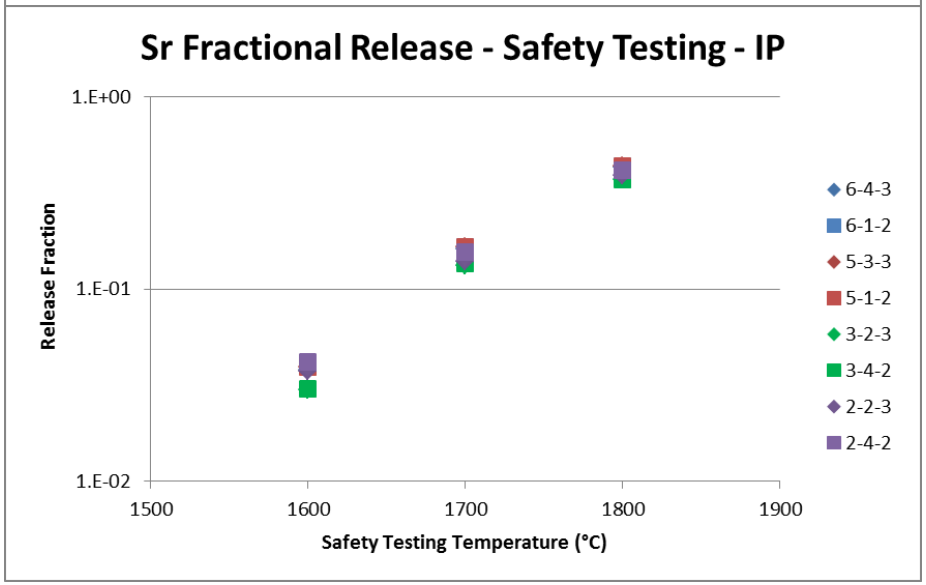



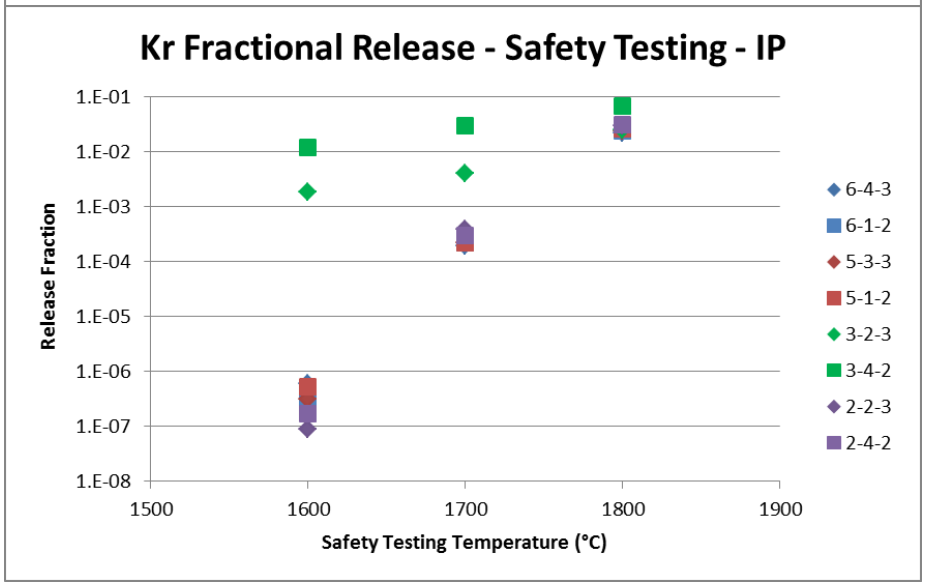



# Fractional Release – Safety Testing (IP)

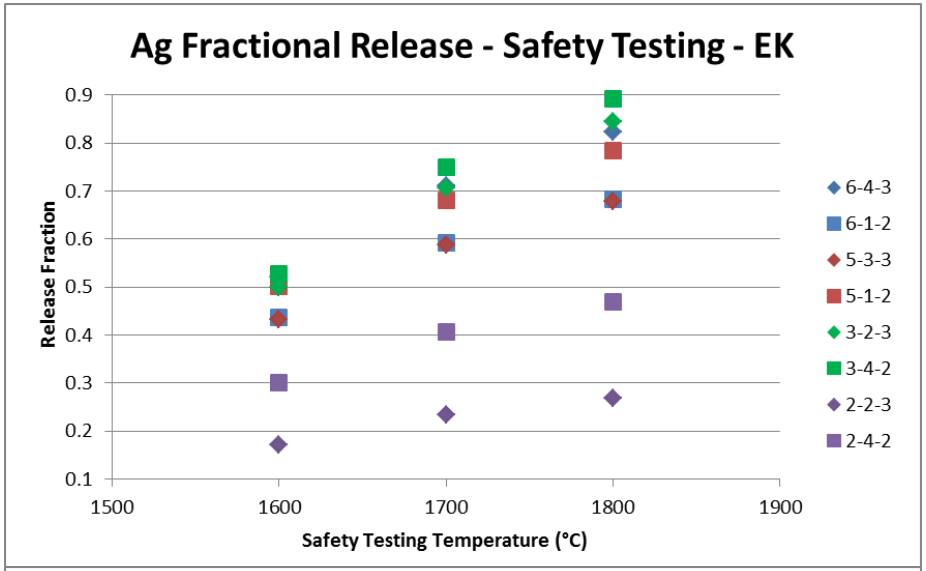


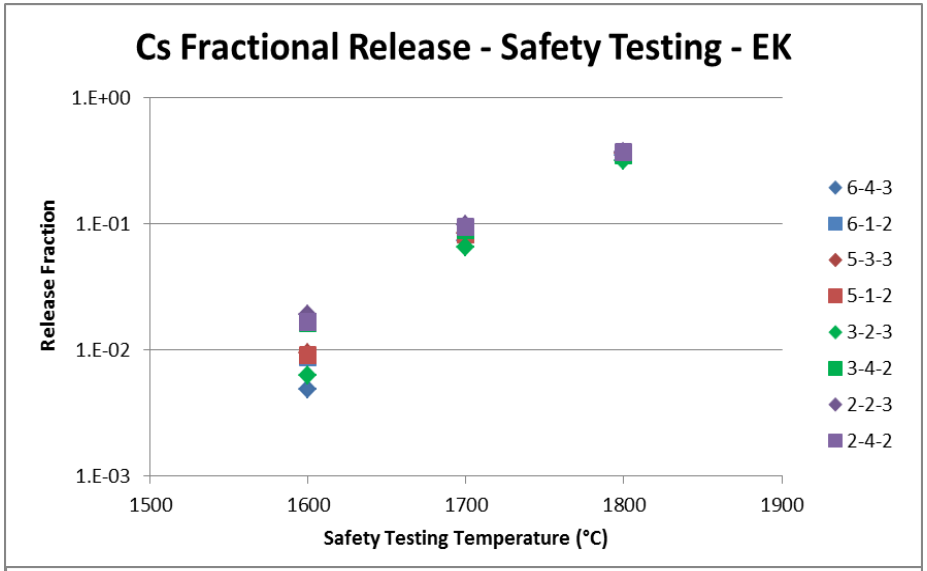



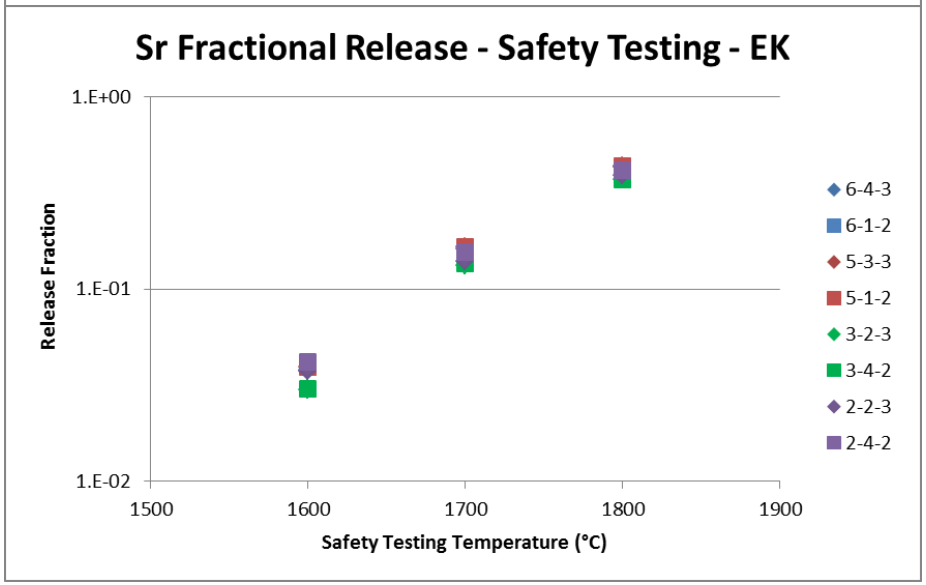



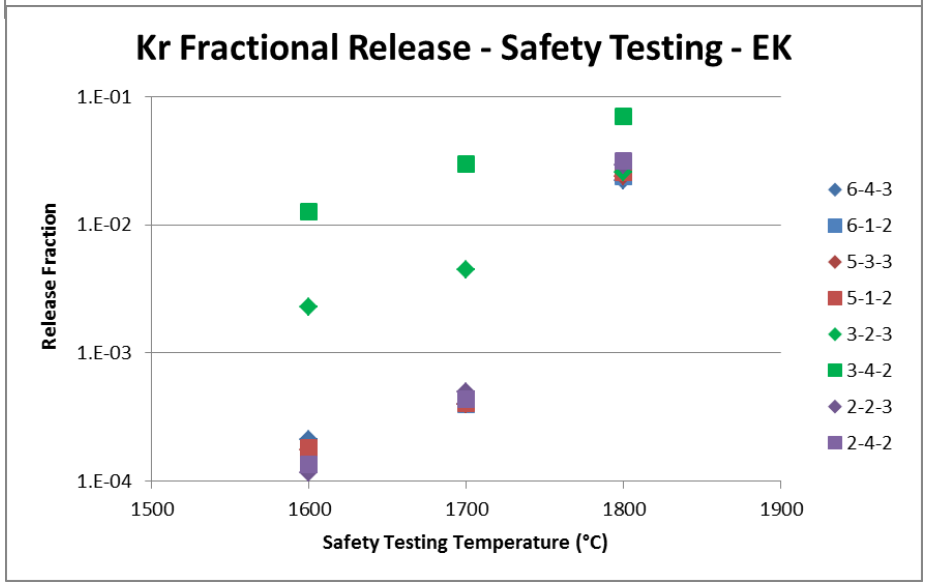



# Fractional Release – Safety Testing (EK)

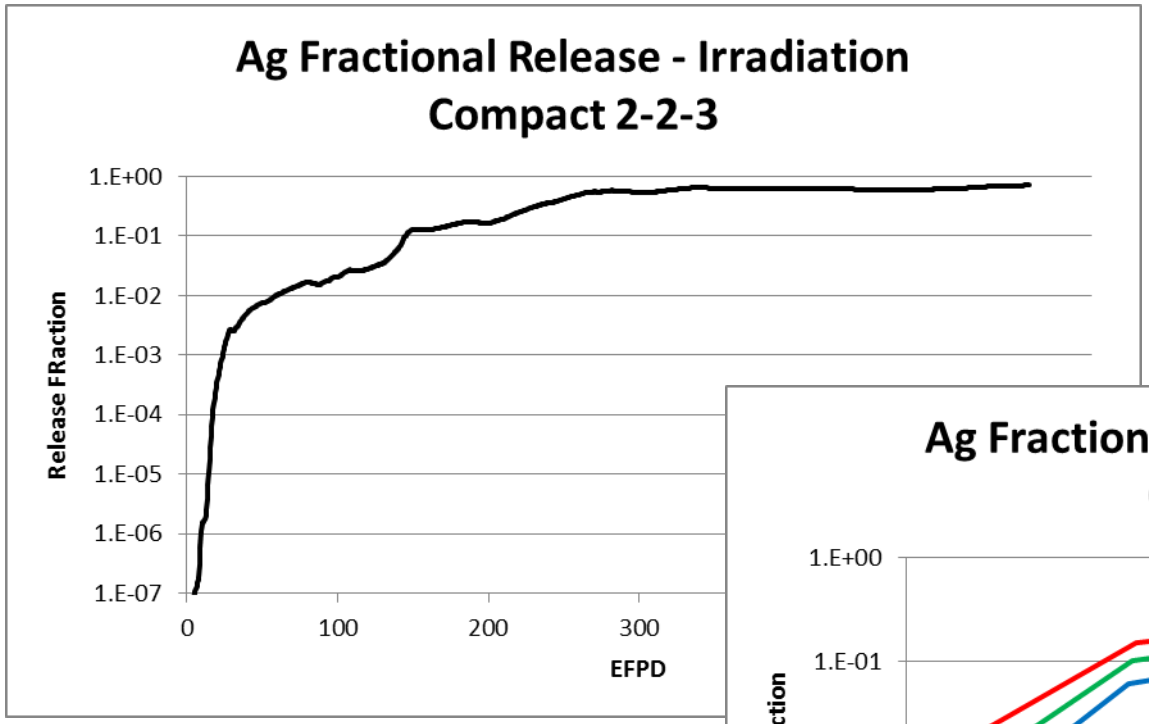


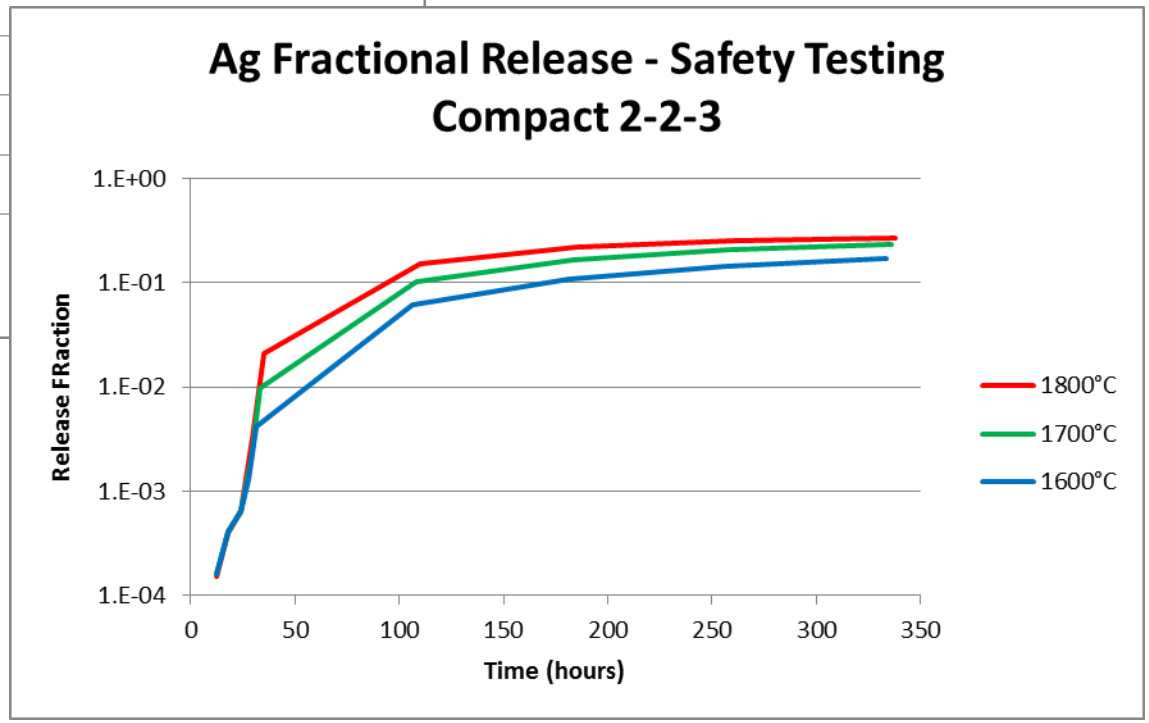



# Fractional Release



# *Fractional Release – Summary*

- Release fraction increases with temperature
  - Increased pressure
  - Increased diffusivity

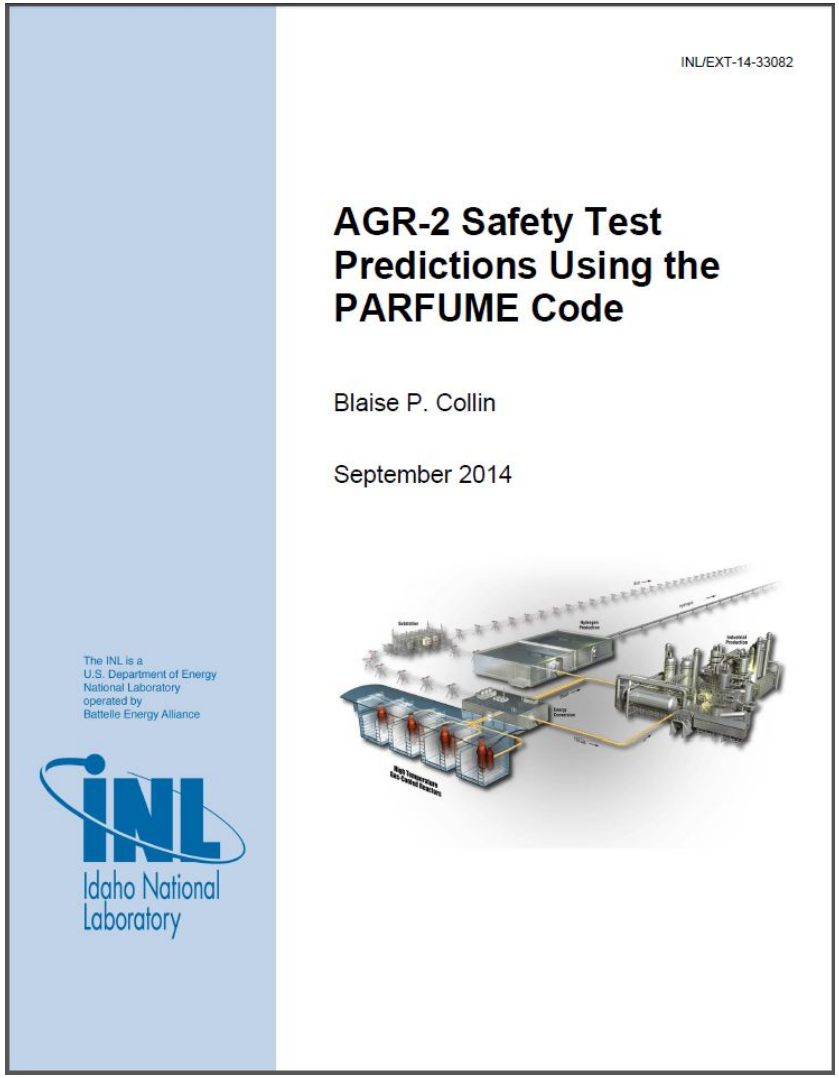
- Ag release fraction 50% - 75% - 90%
- Cs release fraction 1% - 10% - 40%
- Sr release fraction 10% - 20% - 40%
- Kr release fraction UC - 0.02% - 2% (EK ~$3\times10^{-4}$)

- Lessons from AGR-1: PARFUME release during ST over-predicted by 2 to 4 orders of magnitude

# *AGR-2 Safety Test Predictions – Full Report*

**AGR-2 Safety Test Predictions Using the PARFUME Code**

**INL/EXT/14-33082**



INL/EXT-14-33082

AGR-2 Safety Test Predictions Using the PARFUME Code

Blaise P. Collin

September 2014

The INL is a U.S. Department of Energy National Laboratory operated by Battelle Energy Alliance

Idaho National Laboratory

# Questions?

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(208) 526-2217

# Fuel Characteristics (1/2)

| Category | Parameter | Fuel type<br>Mean Value ± Standard Deviation | |
|---|---|---|---|
| | | UCO | $UO_2$ |
| Fuel characteristics | U235 enrichment (wt%) | 14.029 ± 0.026 | 9.600 ± 0.010 |
| | Oxygen/uranium (atomic ratio) | 1.428 ± 0.005 | 2.003 ± 0.005 |
| | Carbon/uranium (atomic ratio) | 0.392 ± 0.002 | N/A |
| | Uranium contamination fraction | $1.59\times10^{-6}$ | $1.57\times10^{-6}$ |
| Particle geometry | Kernel diameter (μm) | 426.7 ± 8.8 | 507.7 ± 11.9 |
| | Buffer thickness (μm) | 98.9 ± 8.4 | 97.7 ± 9.9 |
| | IPyC thickness (μm) | 40.4 ± 2.5 | 41.9 ± 3.2 |
| | SiC thickness (μm) | 35.2 ± 1.2 | 37.5 ± 1.2 |
| | OPyC thickness (μm) | 43.4 ± 2.9 | 45.6 ± 2.4 |
| | Particle asphericity @ SiC (aspect ratio) | 1.037 ± 0.011 | 1.034 ± 0.010 |

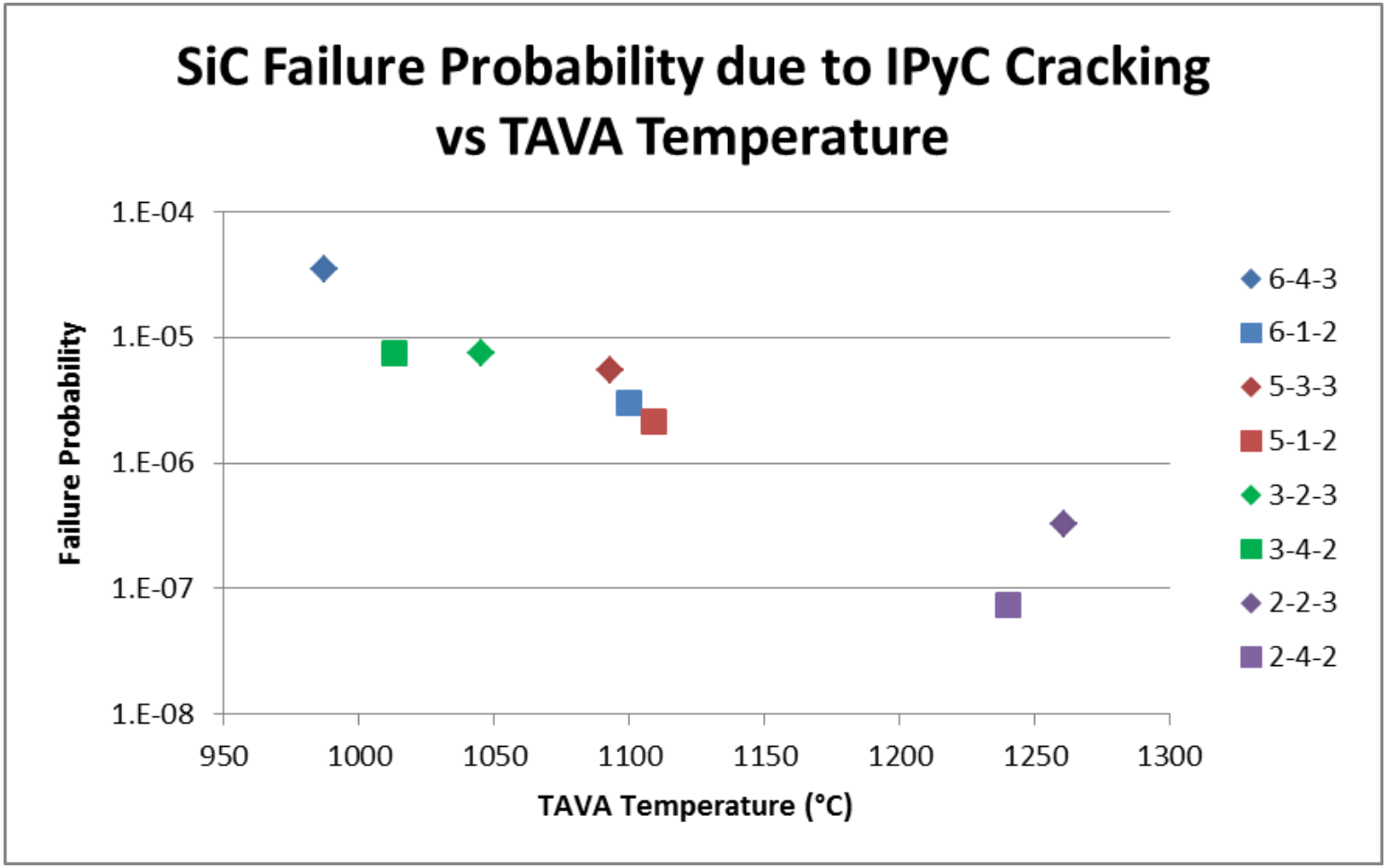
# Fuel Characteristics (2/2)

| Category | Parameter | Fuel type<br>Mean Value ± Standard Deviation | |
|---|---|---|---|
| | | UCO | $UO_2$ |
| Compact characteristics | Diameter (mm) | 12.286 ± 0.005 | 12.269 ± 0.007 |
| | Number of particles per compact | 3176 | 1543 |
| | Compact matrix density (g/cm$^3$) | 1.589 ± 0.005 | 1.680 ± 0.008 |
| Material properties | Kernel density (g/cm$^3$) | 10.966 ± 0.033 | 10.858 ± 0.082 |
| | Buffer density (g/cm$^3$) | 1.05 | 0.99 |
| | IPyC density (g/cm$^3$) | 1.890 ± 0.011 | 1.90 ± 0.05 |
| | OPyC density (g/cm$^3$) | 1.907 ± 0.007 | 1.884 ± 0.004 |
| | IPyC (post compact anneal) BAF | 1.0465 ± 0.0049 | 1.0471 ± 0.0036 |
| | OPyC (post compact anneal) BAF | 1.0429 ± 0.0019 | 1.0365 ± 0.0016 |

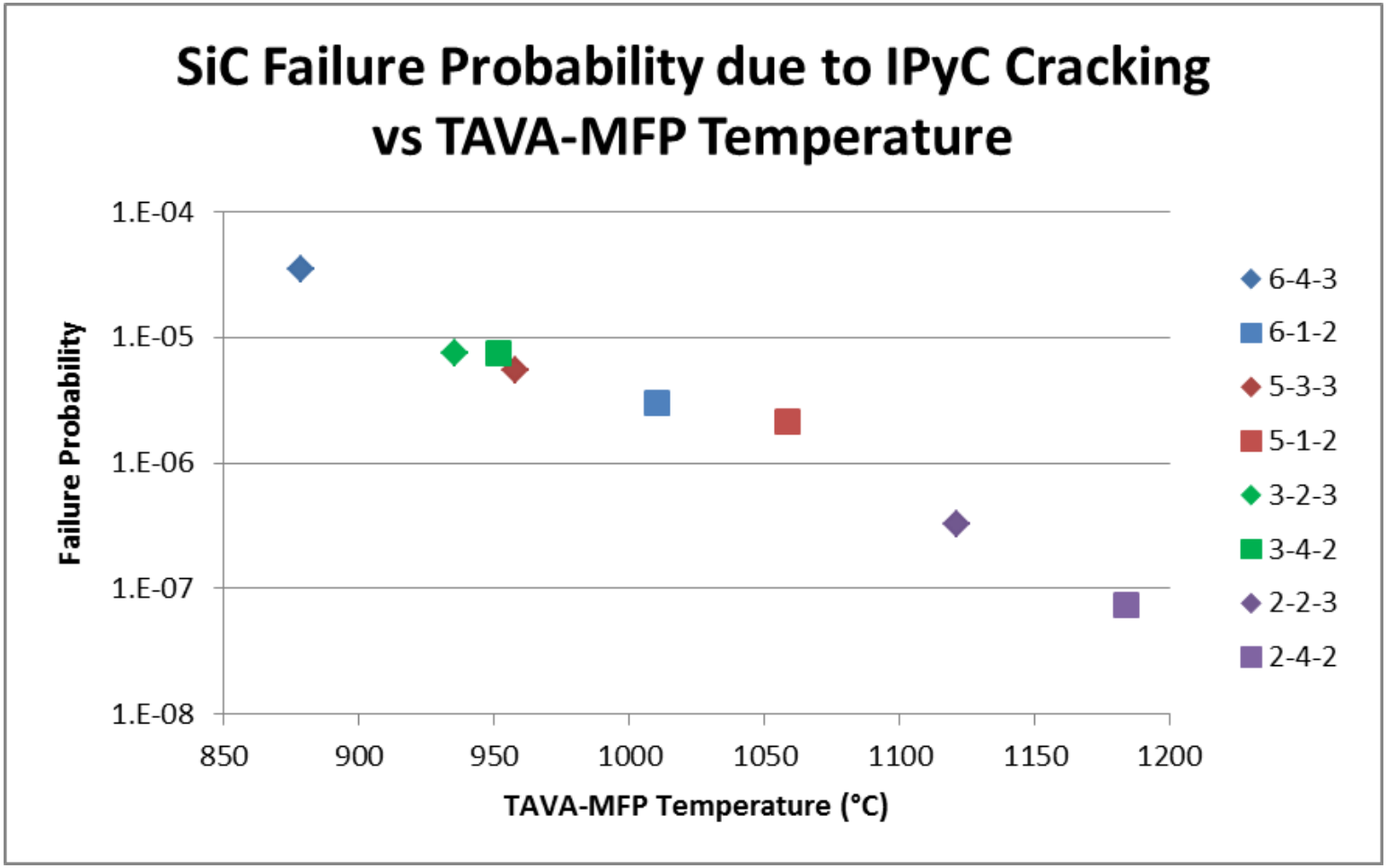
# Diffusion Coefficients

| Species | $D_{0,i}$ ($m^2/s$)<br>$Q_{0,i}$ (kJ/mol) | Kernel | Buffer | IPyC / OPyC | SiC | Matrix graphite | Structural graphite |
|---|---|---|---|---|---|---|---|
| Ag | $D_{0,1}$ | $6.7\times10^{-9}$ | $10^{-8}$ | $5.3\times10^{-9}$ | $3.6\times10^{-9}$ | 1.6 | 1.6 |
| | $Q_{0,1}$ | 165 | 0 | 154 | 215 | 258 | 258 |
| Cs | $D_{0,1}$ | $5.6\times10^{-8}$ | $10^{-8}$ | $6.3\times10^{-8}$ | $5.5\times10^{-14}\times e^{\Gamma/4.5}$ | $3.6\times10^{-4}$ | $1.7\times10^{-6}$ |
| | $Q_{0,1}$ | 209 | 0 | 222 | 125 | 189 | 149 |
| | $D_{0,2}$ | $5.2\times10^{-4}$ | - | - | $1.6\times10^{-2}$ | - | - |
| | $Q_{0,2}$ | 362 | | | 514 | | |
| Kr | $D_{0,1}$ | $1.3\times10^{-12}$ / $8.8\times10^{-15}$ | $10^{-8}$ | $2.9\times10^{-8}$ | 37 / $8.6\times10^{-10}$ | $6.0\times10^{-6}$ | $6.0\times10^{-6}$ |
| | $Q_{0,1}$ | 126 / 54 | 0 | 291 | 657 / 326 | 0 | 0 |
| | $D_{0,2}$ | 0 / $6.0\times10^{-1}$ | - | $2.0\times10^{5}$ | - | - | - |
| | $Q_{0,2}$ | 0 / 480 | | 923 | | | |
| Sr | $D_{0,1}$ | $2.2\times10^{-3}$ | $10^{-8}$ | $2.3\times10^{-6}$ | $1.2\times10^{-9}$ | $10^{-2}$ | $1.7\times10^{-2}$ |
| | $Q_{0,1}$ | 488 | 0 | 197 | 205 | 303 | 268 |
| | $D_{0,2}$ | - | - | - | $1.8\times10^{-6}$ | - | - |
| | $Q_{0,2}$ | | | | 791 | | |

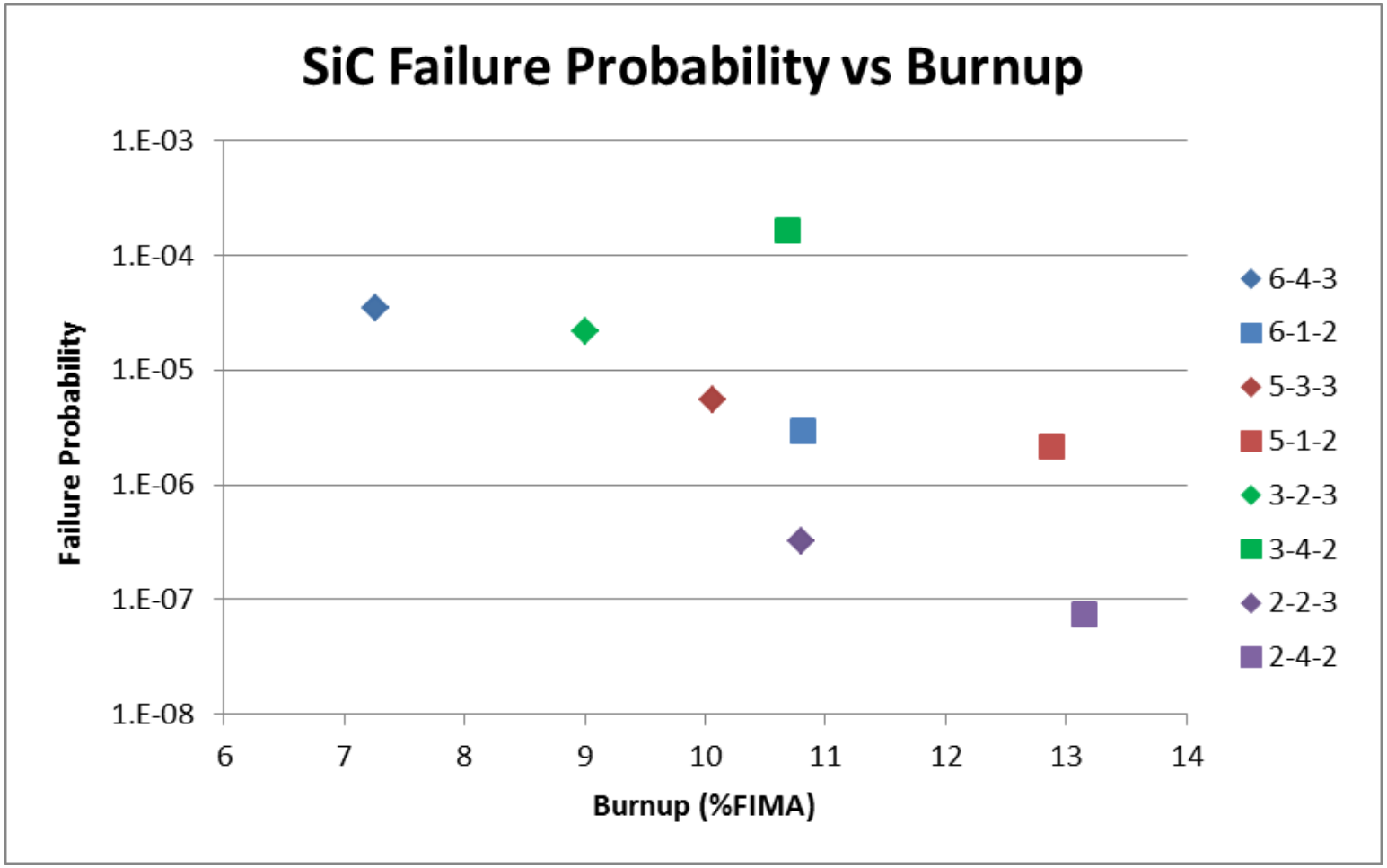
# Failure Probability – Irradiation



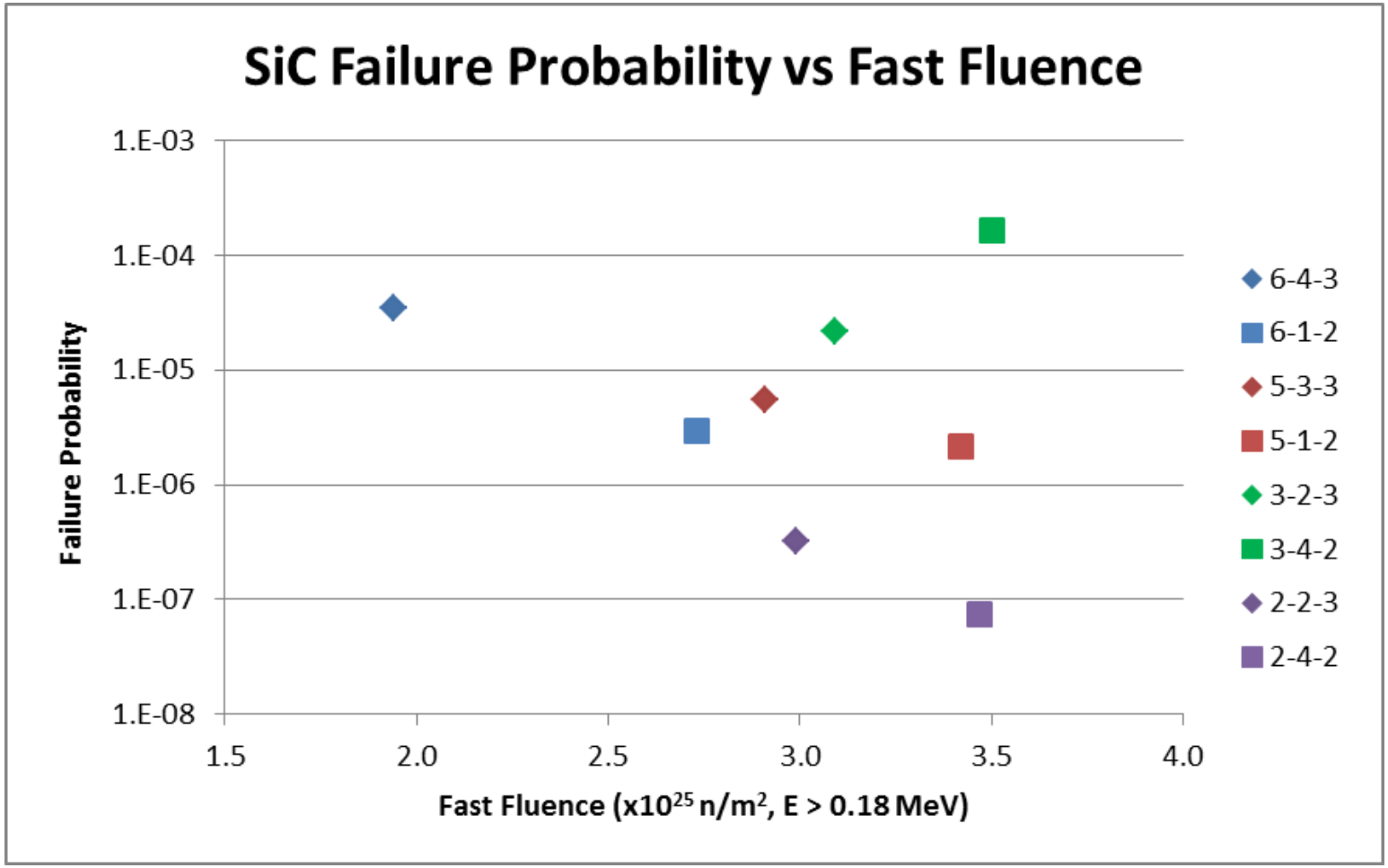
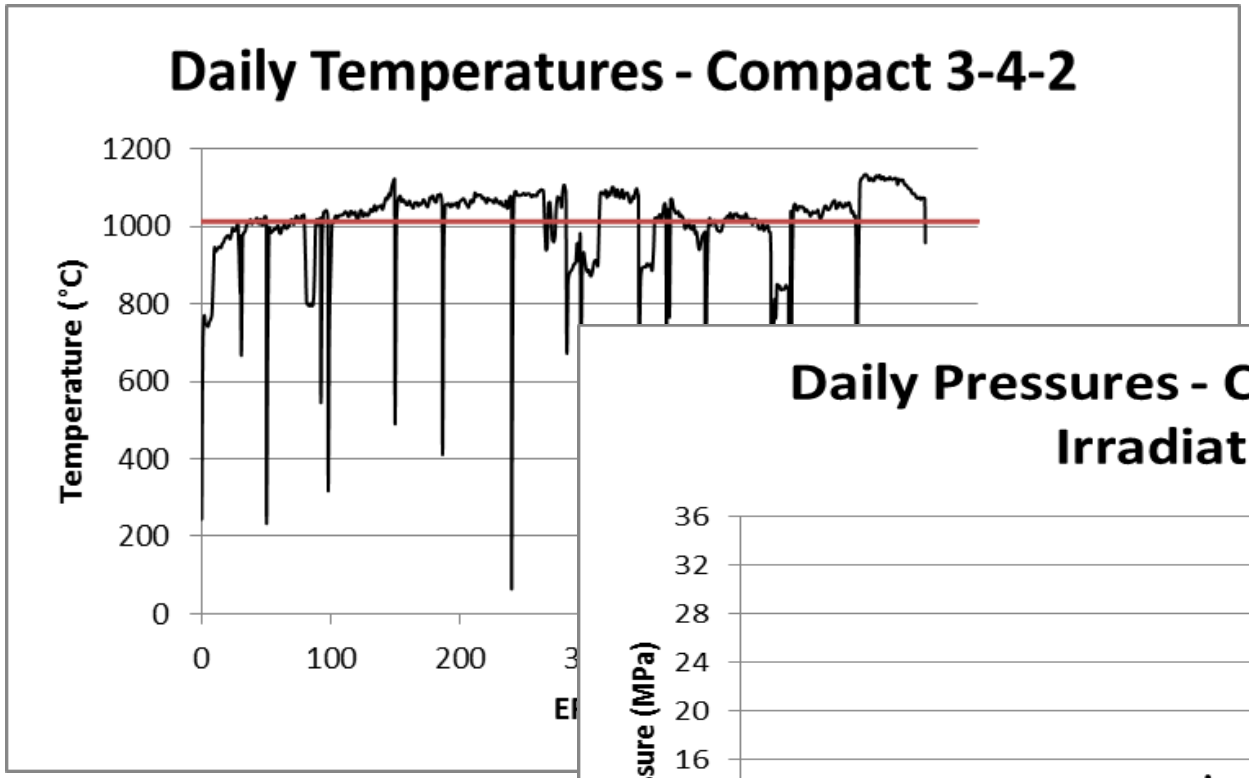
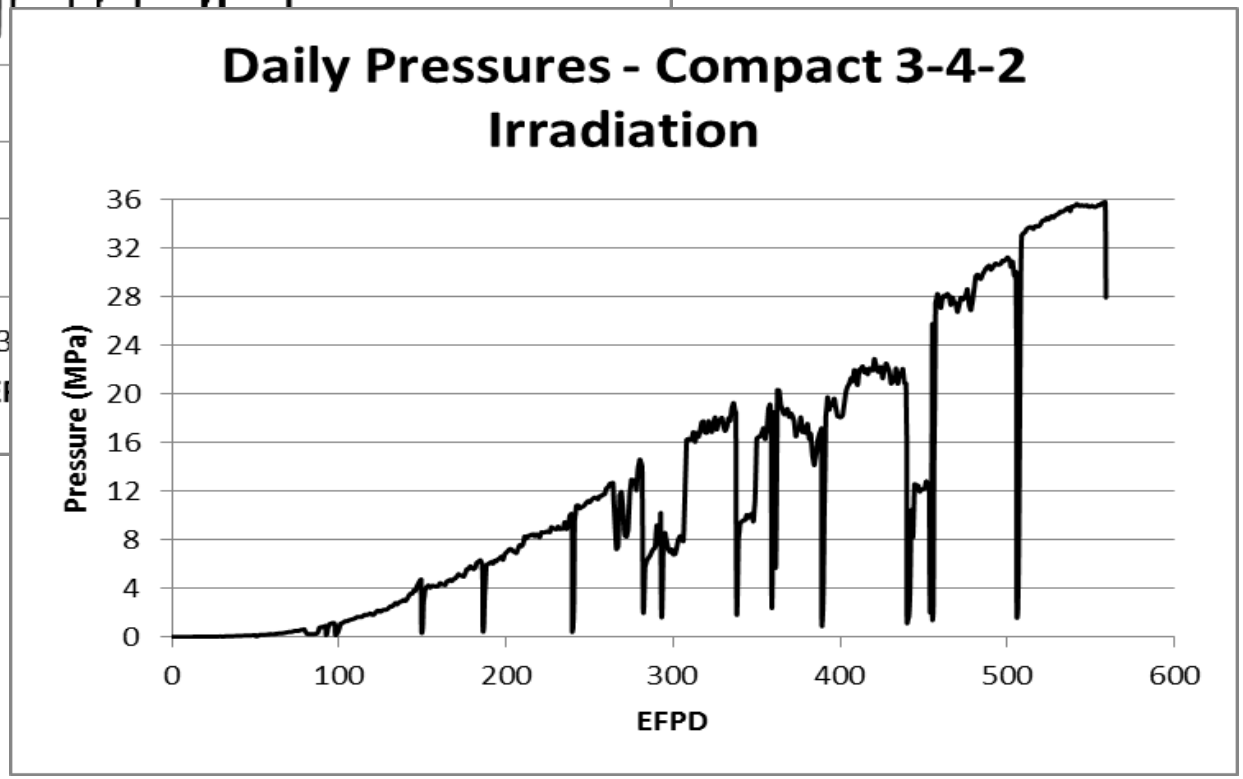
# Failure Probability – Irradiation



# Failure Probability – Irradiation



# Failure Probability – Irradiation



# Failure Probability – Irradiation