

WP5.3: FRACTURE MODELS FOR RPV AND FOR THE IASCC OF INTERNALS

The logo for wood., consisting of the word "wood." in a bold, dark blue, lowercase sans-serif font.

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(Prepared with extensive contributions from SOTERIA WP5.3)



- ❑ This presentation provides an overview of the completed activities within the SOTERIA Project related to fracture predictions.

- ❑ The aim is to provide an overview of Local Approach (LA) process and the various fracture models (*including Irradiation Assisted Stress Corrosion Cracking, IASCC*) being considered.

- ❑ The questions at the start of the project were to consider:
 - The influence of plasticity in cleavage fracture,
 - Improve the understanding of outlying results / materials inhomogeneity and its influence on the cleavage fracture predictions,
 - Experimental validation / comparison of models.
 - Improve modelling of the IASCC process.

Following information taken from following reports, as well as additional work.

- ❑ Di5.1 – Treatment of plasticity in existing fracture models (CEA) **[M12]**
 - Provide an overview of the way that plasticity is included in existing fracture models.
 - This will be used to provide advice on potential modifications.

- ❑ Di5.4 – Prediction of crack-tip stress fields and adaptation of fracture models (EDF, CEA) **[M24]**
 - Consider detailed, state-of-the-art, assessment of the crack-tip stress fields and the effects of plasticity.
 - This will be used to update the Beremin model developed in Perform 60 which may allow a modified Weibull type expression.

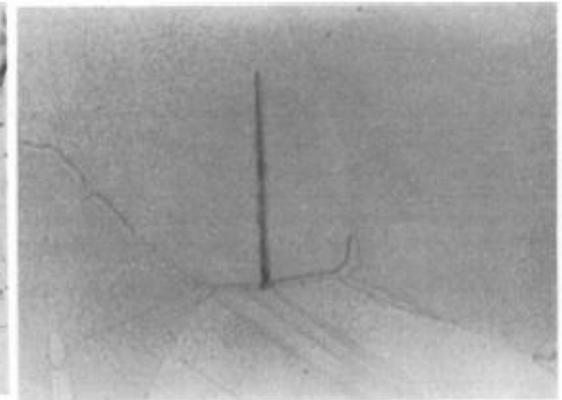
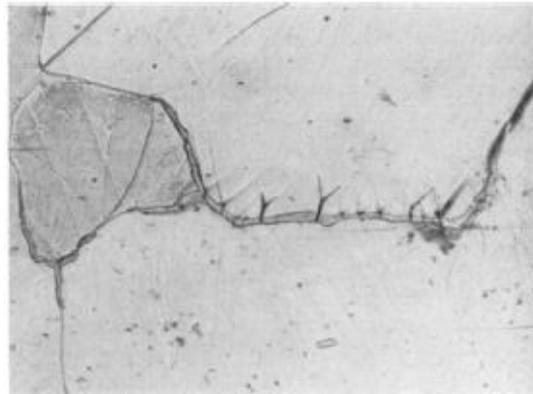
- ❑ Di5.6 – Effect of grain boundary on fracture for RPV (CEA, EDF) **[M36]**
 - Assess mechanisms of crack initiation and propagation related to grain boundary
 - Study influence of spatial heterogeneity of the carbide positions on fracture models

- ❑ **D5.4** - Effect of localised heterogeneities on cleavage fracture (Wood, CEA, AR-G) **[M42]**
 - Consider comparisons against available validation data.
 - Effect of spatial heterogeneity of carbides.
 - Look at outlying results and see if models are able to capture this within expected variations of material properties.

- ❑ These fracture aspects are focused on the estimates of cleavage fracture in ferritic steels and IASCC in austenitic stainless steels, under irradiated conditions.
- ❑ Cleavage fracture is being predicted using a range of approaches, including:
 - the Beremin Model [1],
 - the Bordet Model [2],
 - the JFJ Model [3],
 - the Micro-structurally Informed Brittle Fracture (MIBF) Model [4, 5].
- ❑ IASCC is being modelled through the INITEAC code.
- ❑ Background to these models is included here before an overview of the ongoing activities in SOTERIA is provided.

Background...

- 1) Local Approach (LA) Theory
- 2) Cleavage Fracture LA Models in SOTERIA:
 - 1) Beremin Model
 - 2) Bordet Model
 - 3) JFJ Model
 - 4) MIBF Model
- 3) INITEAC Model for IASCC



Cleavage Fracture Process (1)

- Cleavage fracture is normally considered to include a number of stages to the fracture event. These include:
 - 1) Yielding of the matrix surrounding initiating particles (normally assumed to be carbides, but can be any elastic-brittle particle in the matrix).
 - 2) Brittle particle failure, leading to a micro-crack being formed.
 - 3) Propagation of the micro-crack through the ferritic matrix.

Micro-crack
from plastic
slip [6]

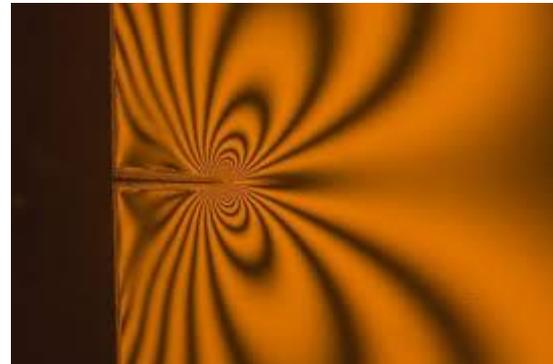


Micro-crack
from shear
stress [6]



- ❑ The use of LA methods to predict fracture generally started from the 1980's (Beremin model).

- ❑ LA models have two main assumptions:
 - 1) Global failure is a weakest link event,
 - 2) The probability of failure is governed by the local mechanical (stress and strain) fields and the local microstructure.



- There is a general formulation that most LA models share to describe the local probability of failure (for a point, i):

$$p_{f,i} = \int_{r_{c,i}}^{\infty} p_{c,i} f(r) dr$$

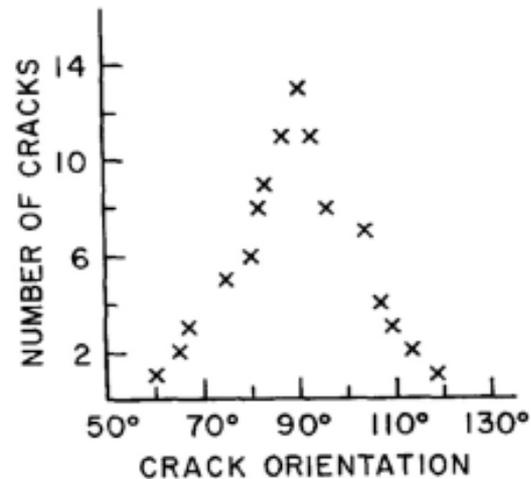
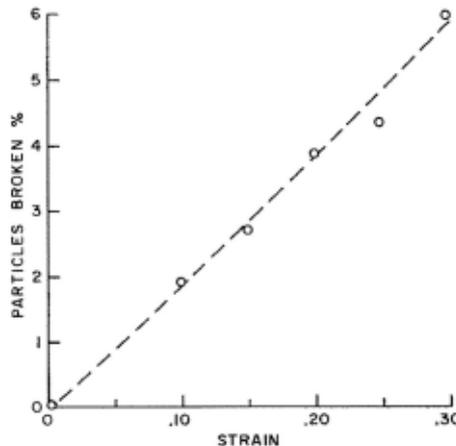
- r is the particle radius, $r_{c,i}$ is the critical micro-crack for propagation, $p_{c,i}$ is the probability of micro-crack nucleation and $f(r)$ is the probability density of the initiators size.
- Assuming all events for i are independent, using the weakest link argument, the global probability of failure is:

$$P_f(V) = 1 - \prod_{i=1}^N (1 - p_{f,i})$$

- N is the number of possible links in the volume V (generally used in finite element analyses with i taken from each integration point).

- $p_{c,i}$, the term that describes the probability of a micro-crack nucleation event captures both:
 - the loading applied to the initiating particles and
 - the subsequent formation of a micro-crack (i.e. stages 1 and 2 previously).
- It is generally observed that:
 - The number of failed particles follows the plastic strain (with cracks forming normal to the loading direction).
 - Larger particles are seen to fail before smaller particles.

Relationship between plastic strain and % particles broken [7]



Frequency of micro-cracks relative to loading orientation [7]

- r_c is the critical micro-crack radius for propagation through the matrix (stage 3 of the cracking process).
- Generally assumed that the cracks behave as Griffith cracks – a crack extends when the elastic strain energy is greater than a critical value (normally assumed to be the surface energy (density) of the matrix, γ_s). Critical stress / critical radius can then be provided as:

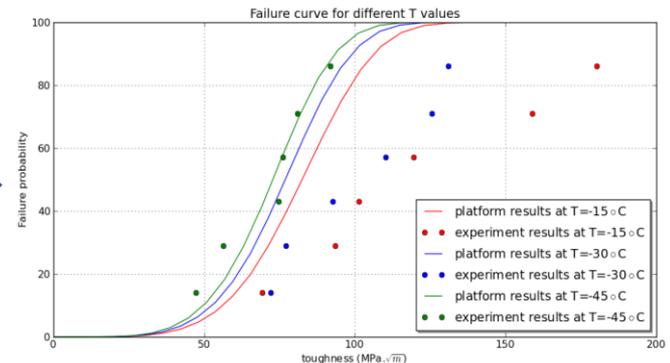
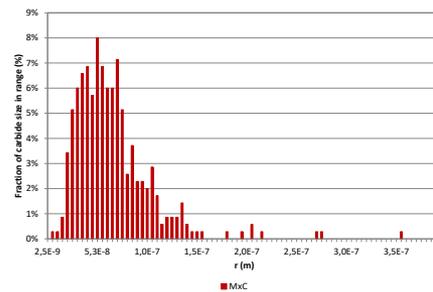
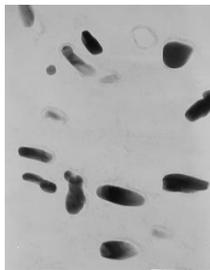
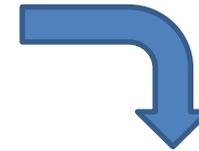
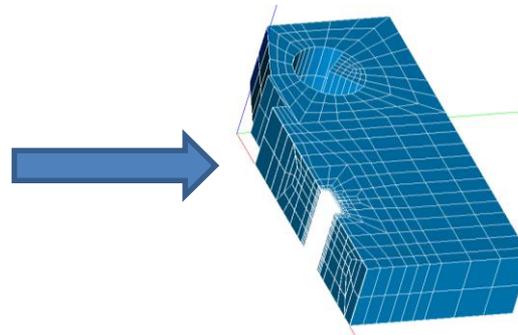
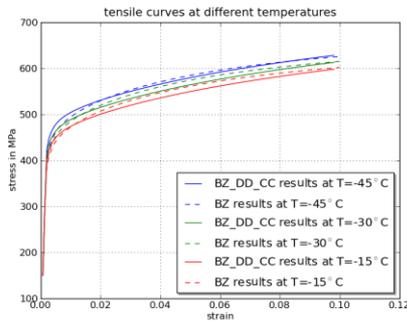
$$\sigma_f = \sqrt{\frac{\pi E \gamma_s}{2(1 - \nu^2)r}} \qquad r_c = \frac{\pi E \gamma_s}{2(1 - \nu^2)\sigma_1^2}$$

where σ_f is the critical stress, E is the materials elastic modulus, ν is Poisson's ratio and σ_1 is the opening/applied stress.

Use of LA models

- ❑ To consider final stage of multi-scale modelling – fracture;
 - Review effect of plasticity on cleavage fracture models,
 - Improve understanding of variation / outlying results,
 - Further experimental validation / comparison of models.

Tensile Curves



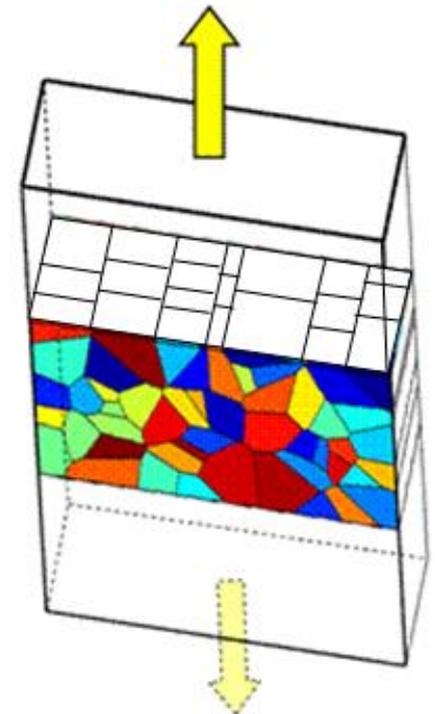
CI Distributions

- ❑ The LA method is well established and many models follow the same underlying assumptions.
- ❑ The Beremin model was initially developed and is still widely used.
- ❑ Further models have looked to improve different aspects of this:
 - How to include plasticity in the nucleation process (Bordet).
 - How to best include plasticity / blunting in the micro-crack propagation (JFJ).
 - Ability to include a measured particle distribution (JFJ & MIBF).
 - How to better account for stress variability (MIBF).
- ❑ *Worth noting that further models (WST, Bernaeur etc) are also available (with slightly different assumptions).*



Predicts nucleation, propagation and coalescence of IASCC

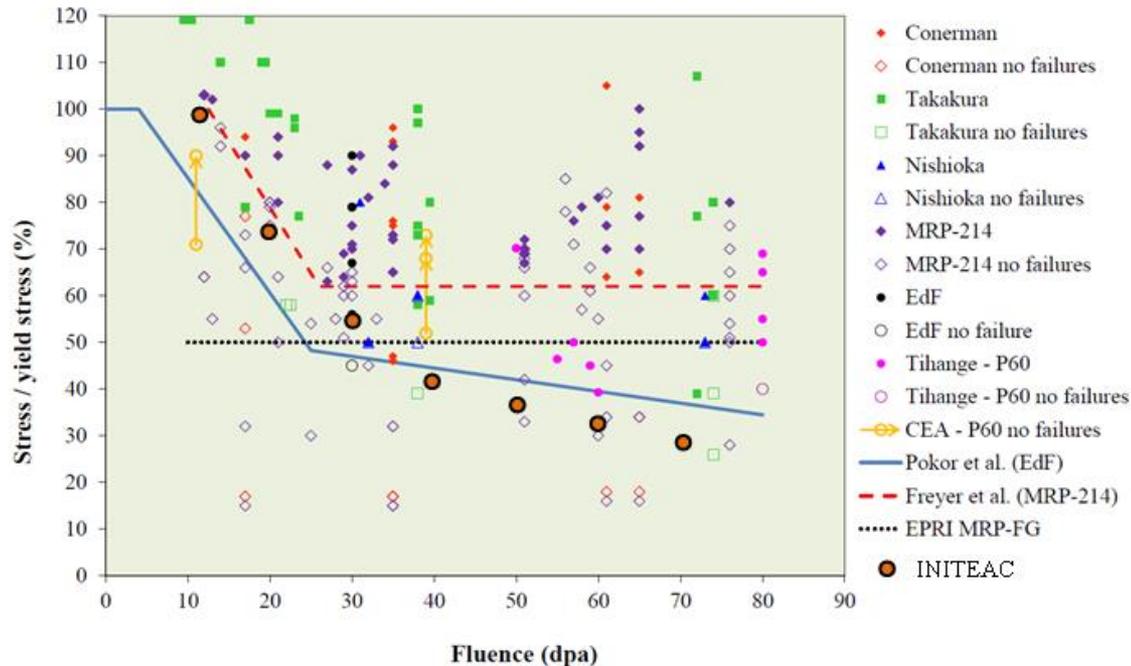
- ❑ Continuum scale modelling (2.5 D)
- ❑ The model continually assesses:
 - Likelihood of crack nucleation
 - Where cracks occur
 - Rates of small and long crack growth
 - Crack coalescence
- ❑ Capable of modelling SCC by internal oxidation or slip dissolution
- ❑ Parameters
 - User configurable GB properties (grain info, Si, Cr)
 - User configurable rules by which GB properties affect damage propagation on GB's
 - Stochastic crack development
 - Input: time profile of stress
 - Outputs: Crack maps & histogram of crack lengths



INITEAC (II) – Typical Results



- ❑ Test results plotted in space defined by test stress / yield for different fluence's.
 - Open symbols no cracking observed. Cracking seen in closed symbols.
- ❑ INITEAC – previous findings:
 - Low dose threshold slope reproduced
 - Reduced threshold slope at higher dose

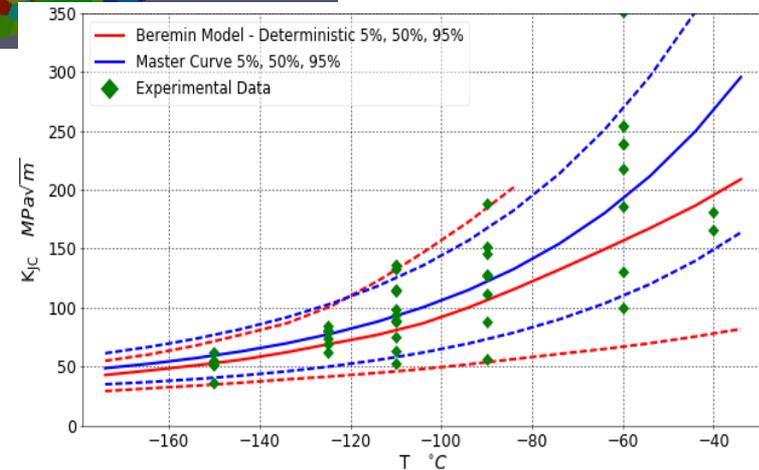
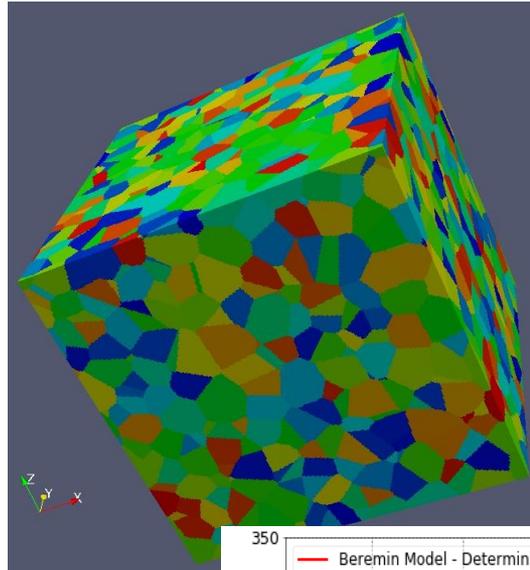


Original plotted data from SCK-CEN/CEA P60 D2-1.7



Activities in SOTERIA

- 1) LA Fracture Models:
 - 1) Plasticity in cleavage fracture,
 - 2) Outlying results,
 - 3) Experimental validation / comparison of models.
- 2) INITEAC Model for IASCC
- 3) Summary



Main objective is to develop micro-structurally informed models for the final stage of the multi-scale simulation process.

This means there is a need to use, better understand and develop the process to model fracture. As noted this relates to:

- Fracture Models for RPV – This typically uses a range of Local Approach models to predict the cleavage fracture toughness.
- Fracture Models for Internals – In SOTERIA this is linked to the INITEAC code for IASCC.



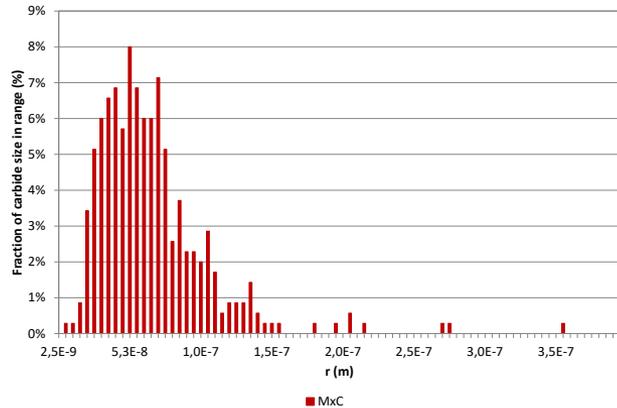
EFFECT OF PLASTICITY

Review effect of plasticity on cleavage fracture models

- ❑ **Review of the treatment of plasticity in existing fracture models**

- ❑ This deliverable conducted a review of different brittle fracture models while focussing on different items:
 - How do they model the nucleation of the micro-defects that will lead to cleavage?
 - How do they model the propagation of these micro-defects towards a macroscopic crack?
 - How are the initiation sites for these micro-defects modelled?
 - What role does plastic strain play in the various assumptions of the model?

Plasticity in LA Models (2) (CEA)



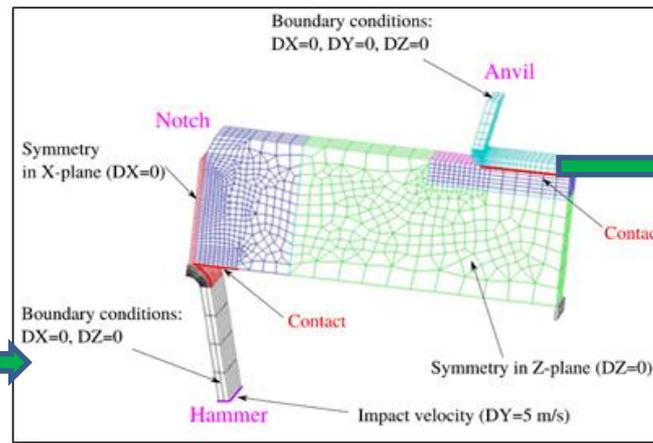
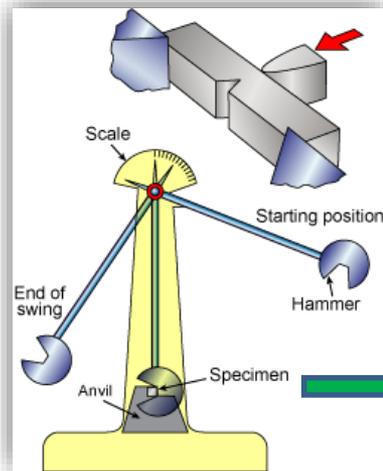
Carbide size distribution		Nucleation		Propagation	
Non explicit power law β/r^α	Beremin	Plasticity induced	All	Griffith	All except Promethey
	Mod Beremin		Promethey	Deterministic propagation	Promethey
	Bernauer CN	Continuous nucleation	Bordet	Truncating	Bordet
	Bernauer DBT				
Bordet					
Explicit asymptotic power law	MIBF	Continuous nucleation	Bernauer CN	Blunting	JFJ
		Energy density	WST		
Lee	MIBF	Energy density	JFJ		
Jayatilaka	WST	Debonding of carbides	Bernauer DBT		
	MIBF				
Ortner	JFJ	Ductile propagation			
	MIBF	GTN		Bernauer DBT	
	(Mathieu)	Crystal plasticity			
Normalized power law	MIBF	Bainitic microstructure		MIBF	
Explicit carbide population	Mathieu	Explicit bainitic microstructure		Mathieu	

It has been shown that all models are compatible with the MIBF model (which also allows crystal plasticity to be considered).

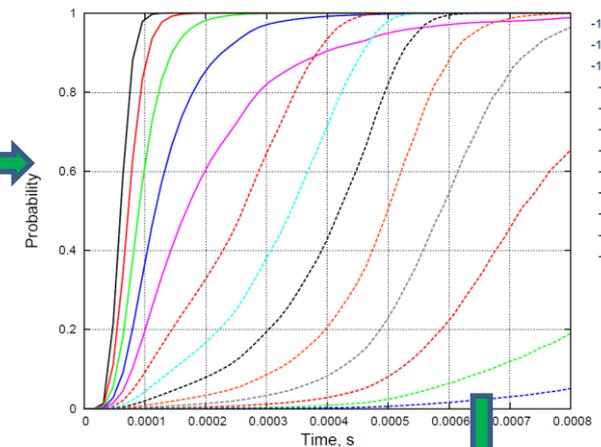


Including Ductile Damage in Prediction (EDF)

- ❑ Modelled Charpy test with elastic-viscoplastic behaviour for brittle fracture and post-processing for cleavage with Beremin model
- ❑ Similar to exercise considered.

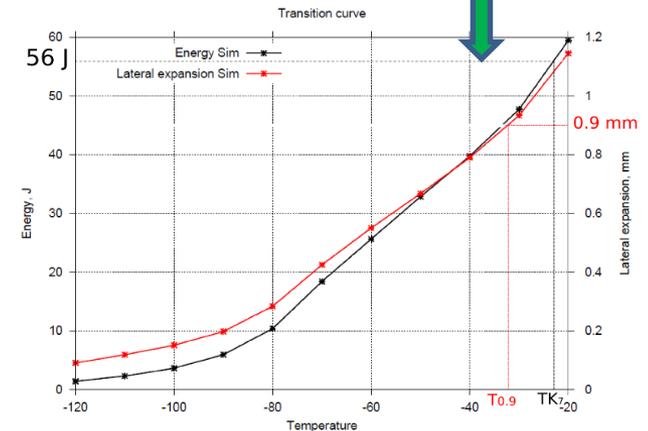


Probability of failure P_f vs. t for different T



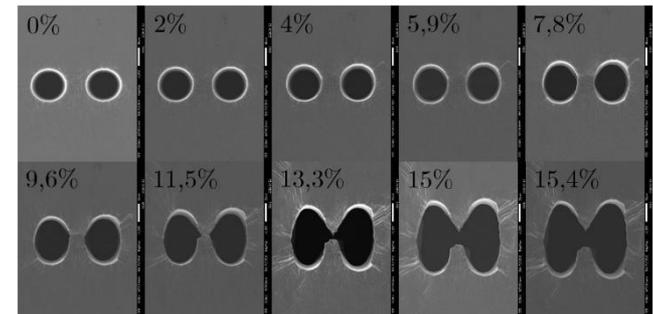
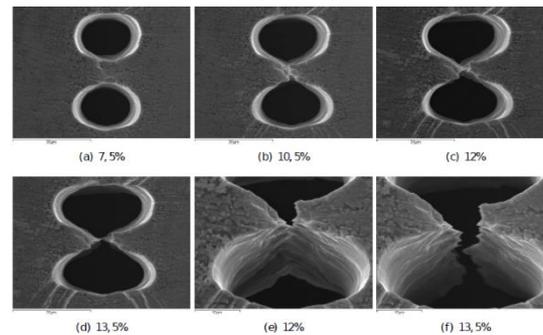
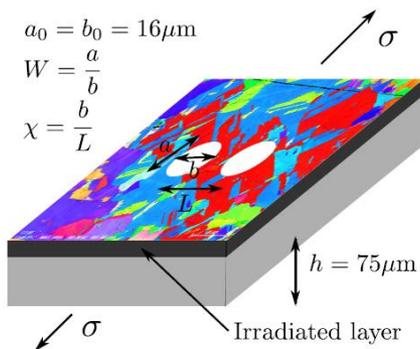
- ❑ Range of assumptions for material properties
- ❑ Promising results, and good prediction of ΔT
- ❑ Looking to introduce the model of the ductile tearing with the use of Gurson model to be able to construct the full DBTT curve (in progress)

DBTT curve



Void Growth and Coalescence (CEA)

- ❑ To provide experimental data on void growth and coalescence in irradiated materials. These data would also be useful to calibrate constitutive equations for irradiated austenitic stainless steels.
- ❑ Ion-irradiated thin tensile samples - Focused Ion Beam (FIB) drilling of cylindrical holes. SEM observation of the evolution of void dimensions under tensile loading was performed.



- ❑ Strong dependence of void deformation to crystallographic orientations.
- ❑ Strong influence of activated slip systems on void coalescence.
- ❑ Now in position to progress to stainless steel experiments.

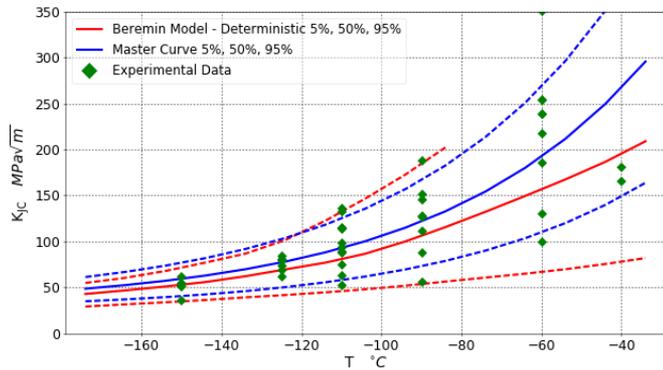
OUTLYING RESULTS

Improve understanding of variation /
outlying results

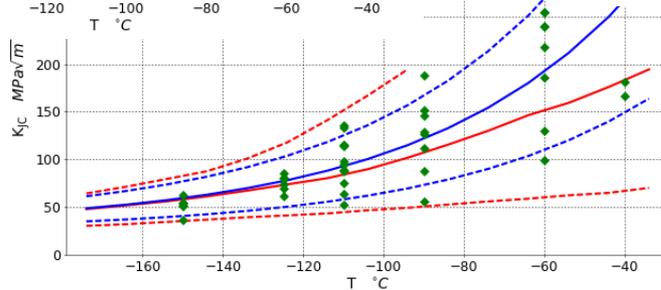
Monte Carlo Implementation of LA Models (Wood)



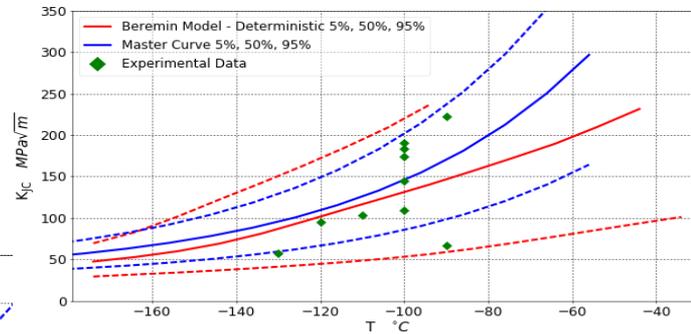
- ❑ To consider variation in the material initiating particles and their impact on fracture toughness. Probabilistic assessments considering localised variation in the calibration parameters of the brittle fracture model(s).
- ❑ Successful use of Beremin and JFJ LA models in a deterministic and probabilistic methods.
- ❑ For reference case materials selected within the programme (parent and weld materials).



NH

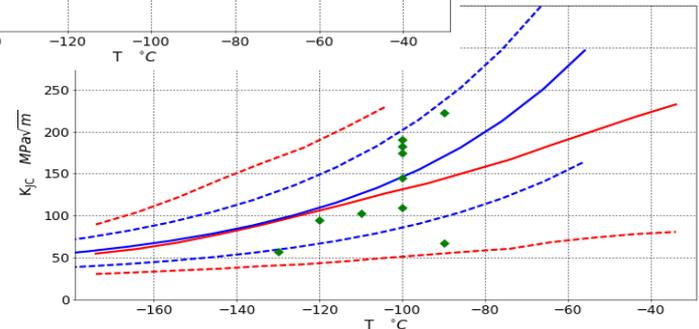


Probabilistic

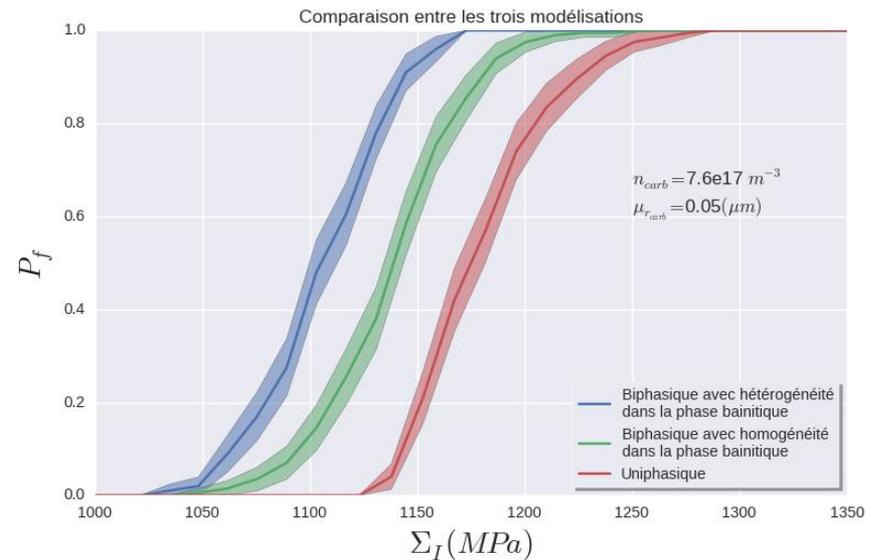
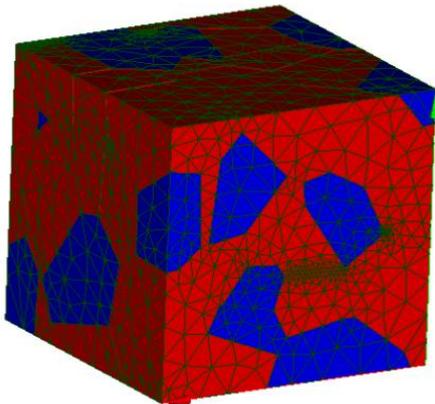


Deterministic

IL



- Determine the influence of the spatial distribution of carbides in a RPV steel in a LA to fracture model, and to assess for the influence of stress heterogeneities at grain boundaries to the onset of brittle fracture.
- The aggregate has 98 grains with a non-regular mesh. Two versions of this aggregate are available:
 - A monophasic one (with only bainite);
 - A biphasic one (with bainite and ferrite):
 - Carbides homogenously in bainite phase.
 - Carbides sample in the bainite phase only and preferentially near the interface.



- ❑ A version of the MIBF model (IG-MIBF) has been developed to specifically consider the effect of grain boundary fracture.
- ❑ This may help explain extreme lower bound fracture data.
- ❑ There is a need to consider:
 - The grain-boundary stress / strain field
 - Estimate of the distribution of initiating particles on the GB
 - An estimate of the critical stress to cause a failure event.

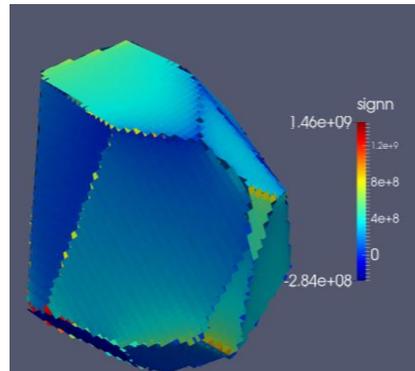
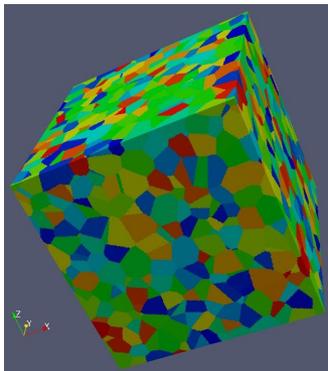
$$P_f(V_p, \Pi) = 1 - \exp \int_{V_p} n_p S_v \cdot \ln(1 - P_g(\sigma_n^* > \sigma_i)) dV$$

Characteristic failure size parameter

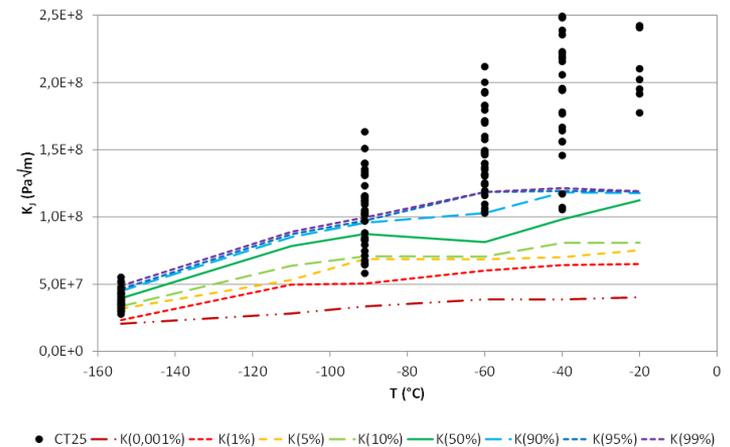
Grain boundary area per volume unit

Grain boundary stress distribution

Intergranular critical stress



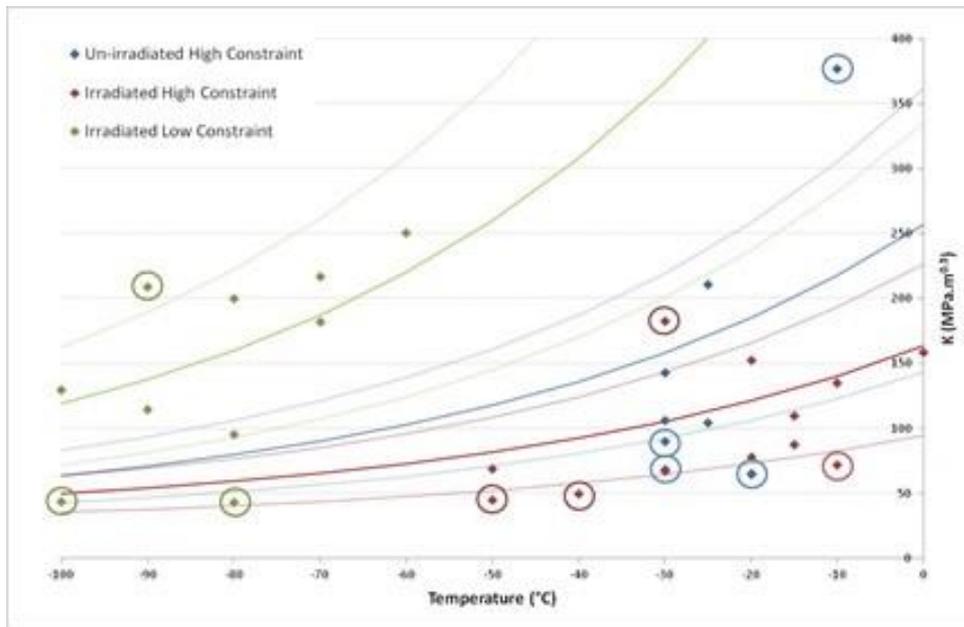
Ductile to brittle transition curve for Euro Material A, for (cleavage) MIBF model combined to (inter-granular) IG-MIBF model with critical stress = 2500 MPa



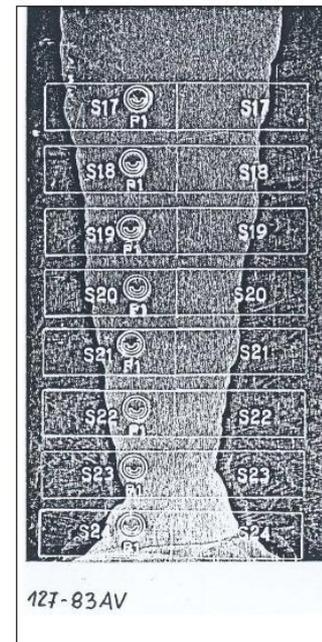
Reference Materials for Comparison (Framatome)

- ❑ Two materials have been considered for validation purposes (parent and weld – referenced as ANP1 [20MnMoNi5-5] and ANP2 [S3NiMo1/OP41 TT]).
- ❑ Chosen as parent conforms to Master Curve, Weld less so. Data readily available from Framatome.
- ❑ Comparisons ongoing (with different LA models identified above)

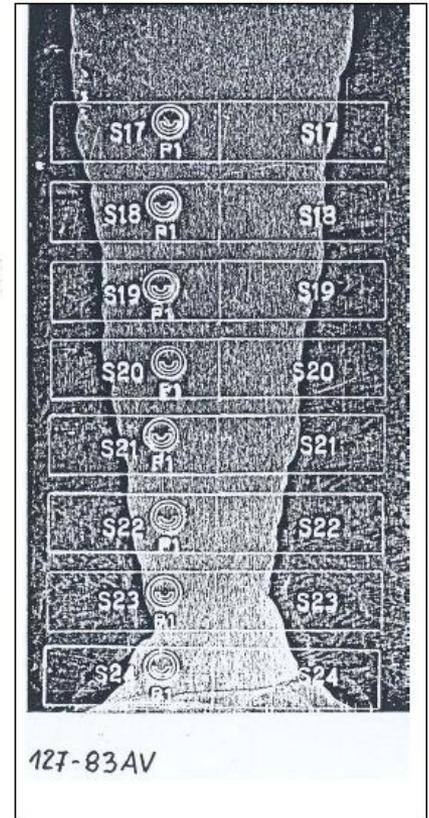
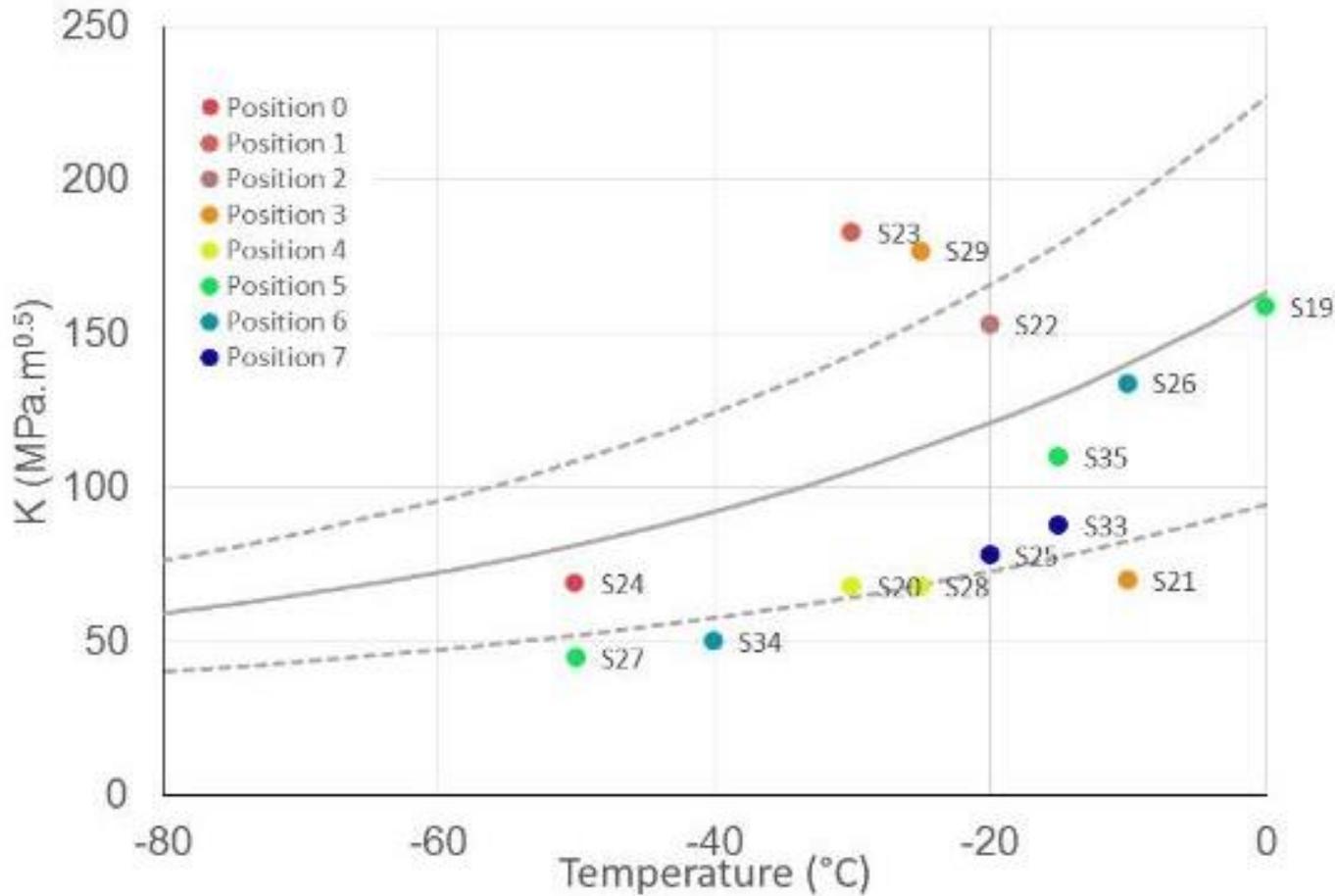
Weld Material Comparison to MC



Extracted locations of weld data



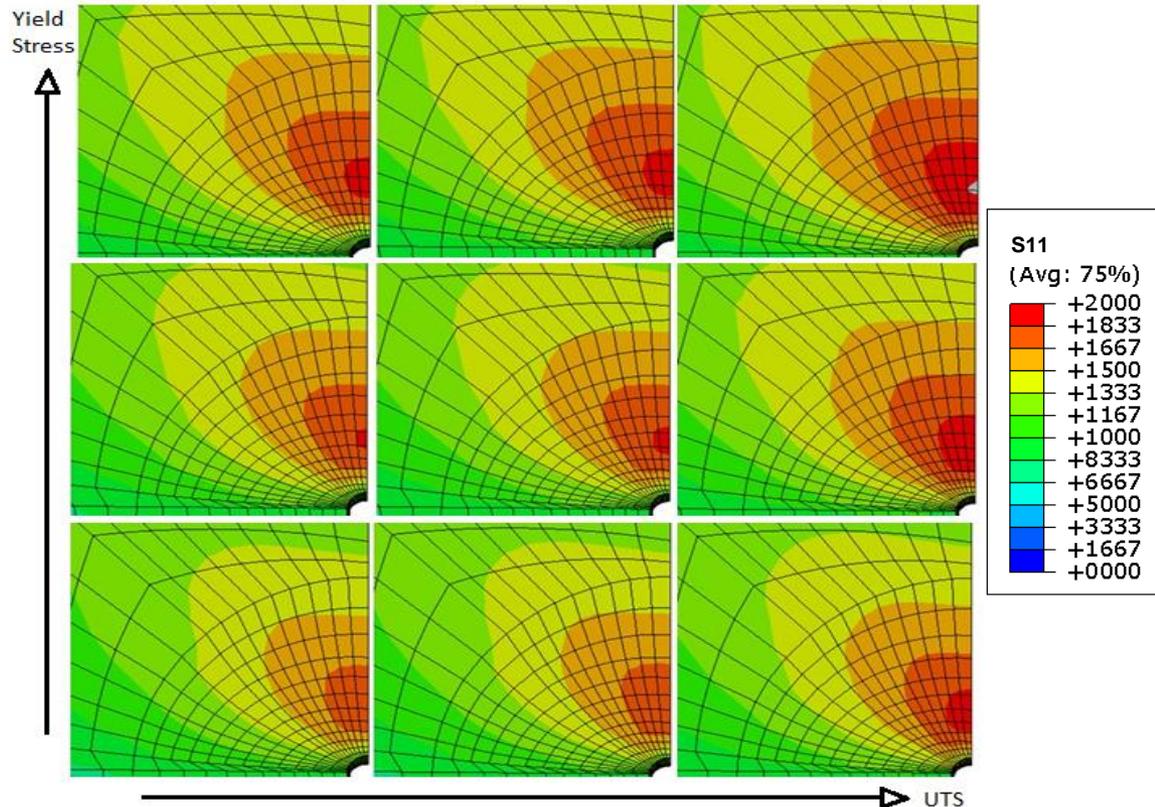
Reference Materials for Comparison (Wood)



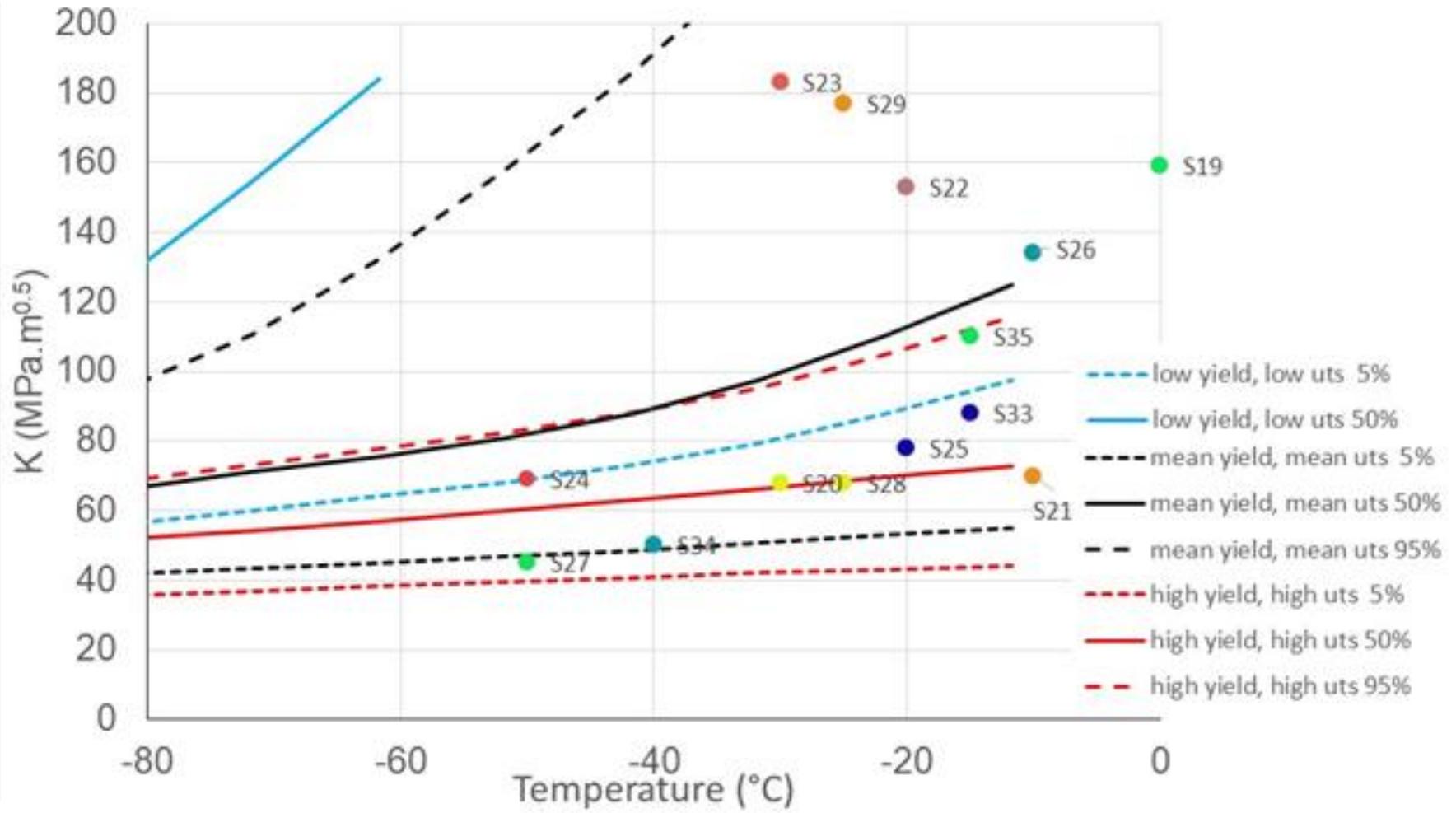
Modelling Tensile Variation (Wood)

[8]

Material	Variable	Lower Bound	Mean	Upper Bound
Un-irradiated	σ_y	0.913	1.0	1.067
	σ_{UTS}	0.983	1.0	1.088
Irradiated	σ_y	0.881	1.0	1.067
	σ_{UTS}	0.926	1.0	1.099



Modelling Tensile Variation (Wood)



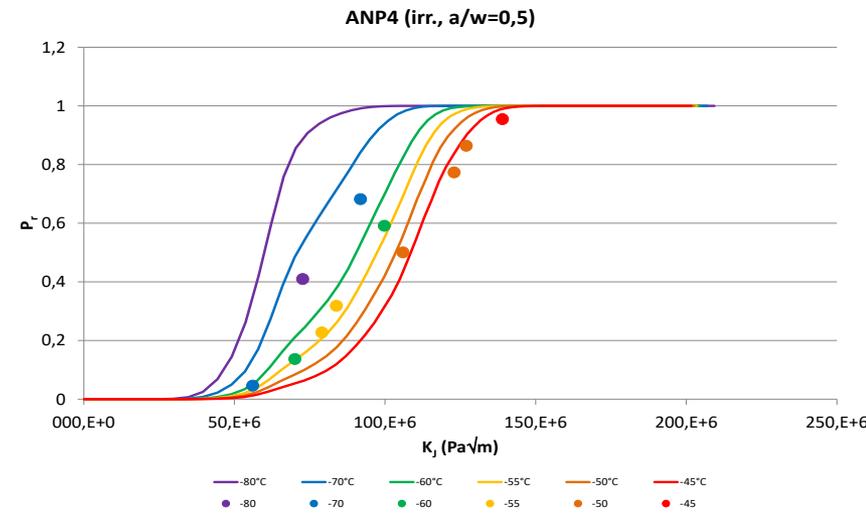
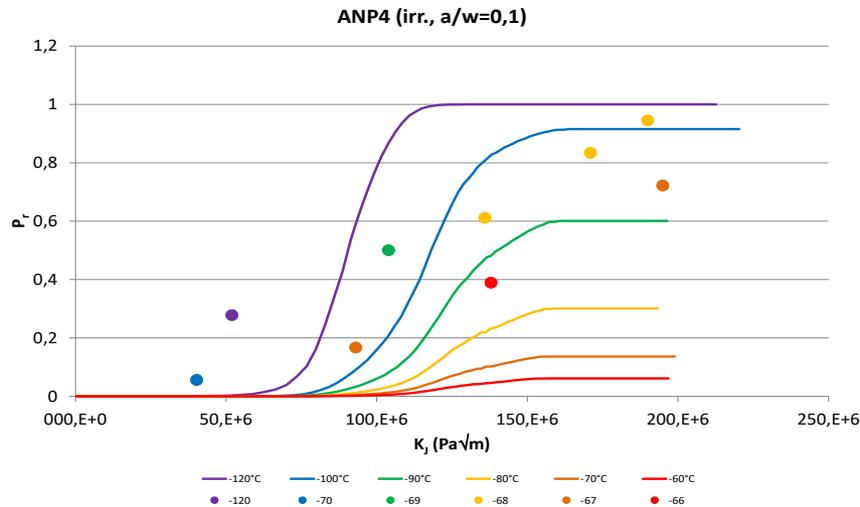
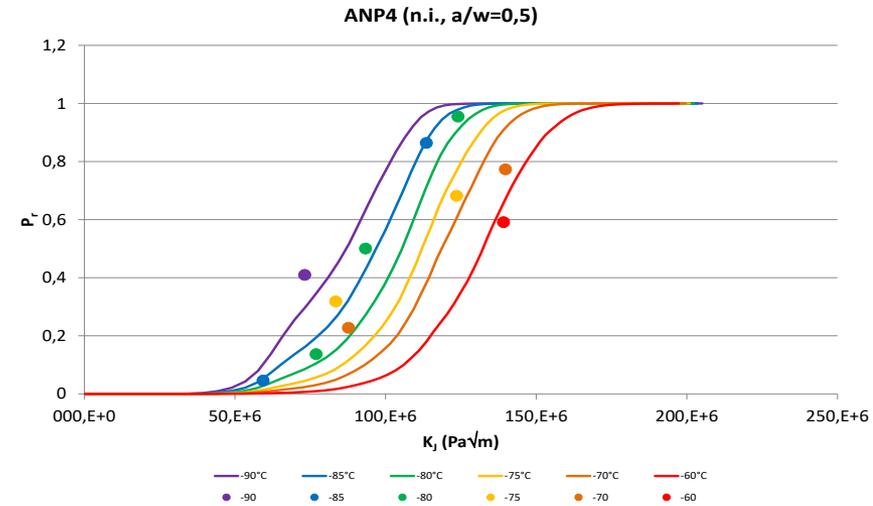
VALIDATION

Further experimental validation /
comparison of models

Application of MIBF to Parent (CEA)



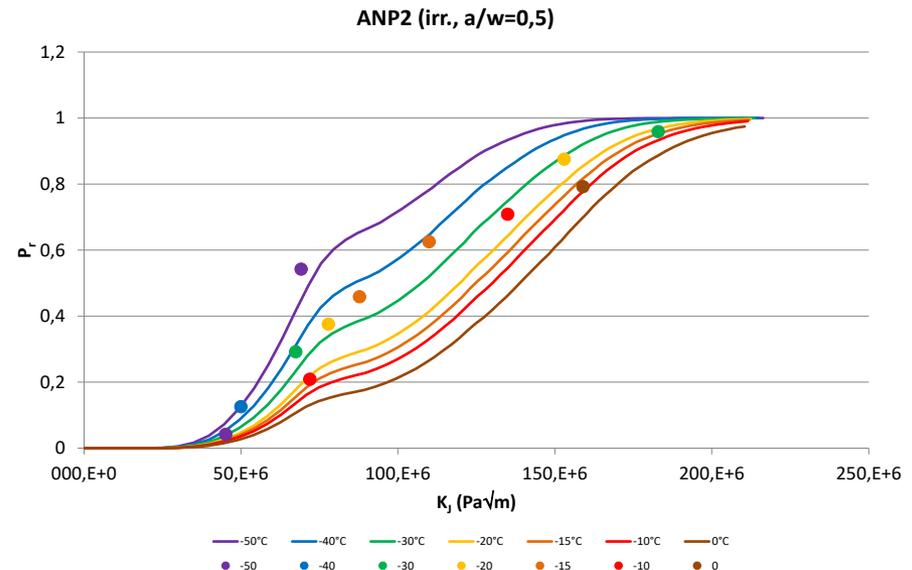
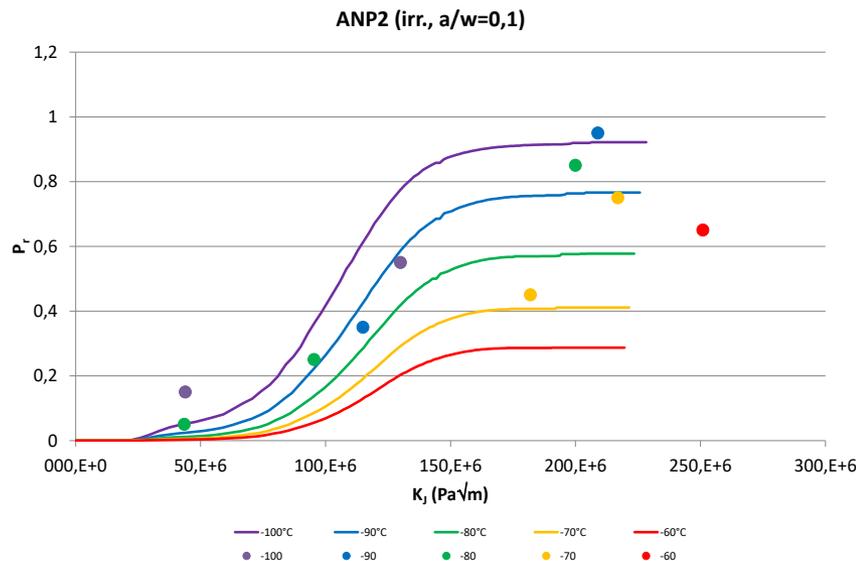
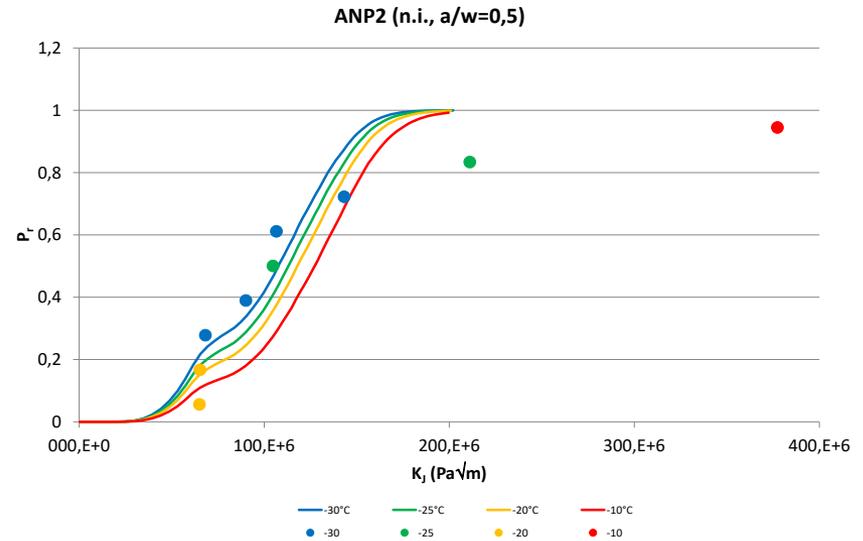
- ❑ MIBF model calibrated against the 3 cases for ANP-1, the calibrated values of γ_f were similar.
- ❑ The value of $\gamma_f = 6.078 \text{ J/m}^2$ was used.
- ❑ Good results were obtained for both high constraint cases, including scatter.
- ❑ The irradiated low constraint case was more difficult to capture, MIBF under-predicted scatter and P_f saturated < 1 .



Application of MIBF to Weld (CEA)

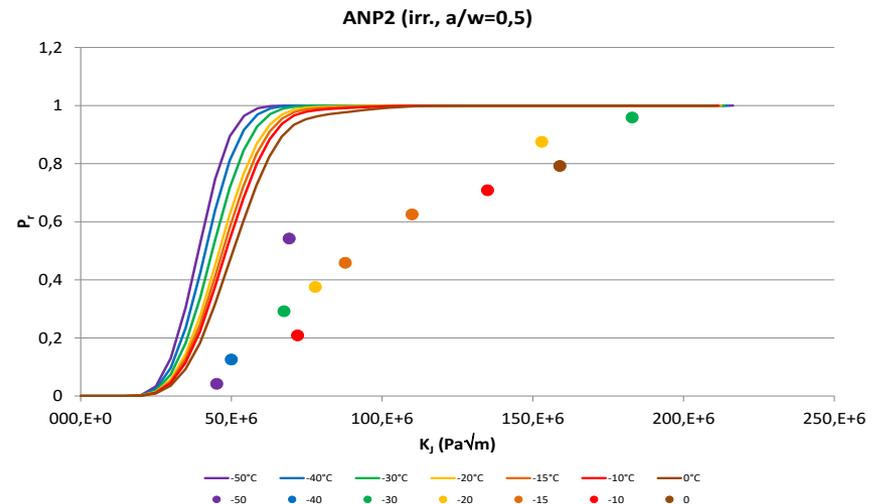
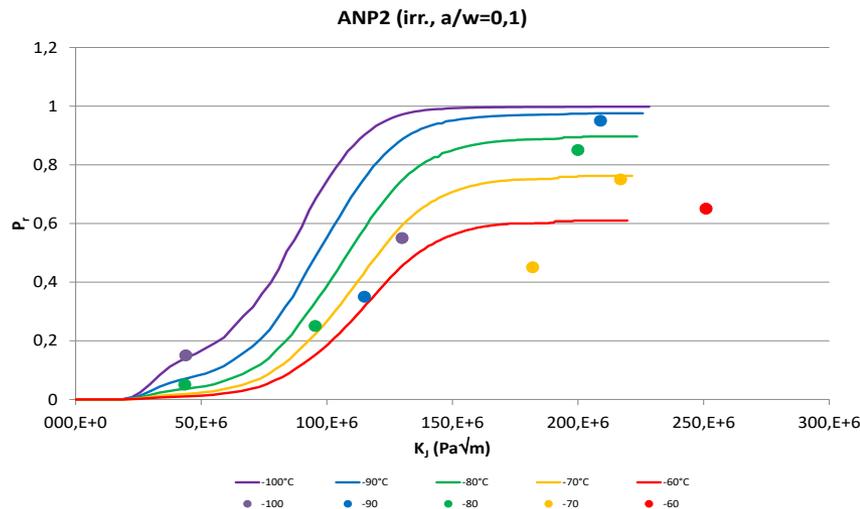
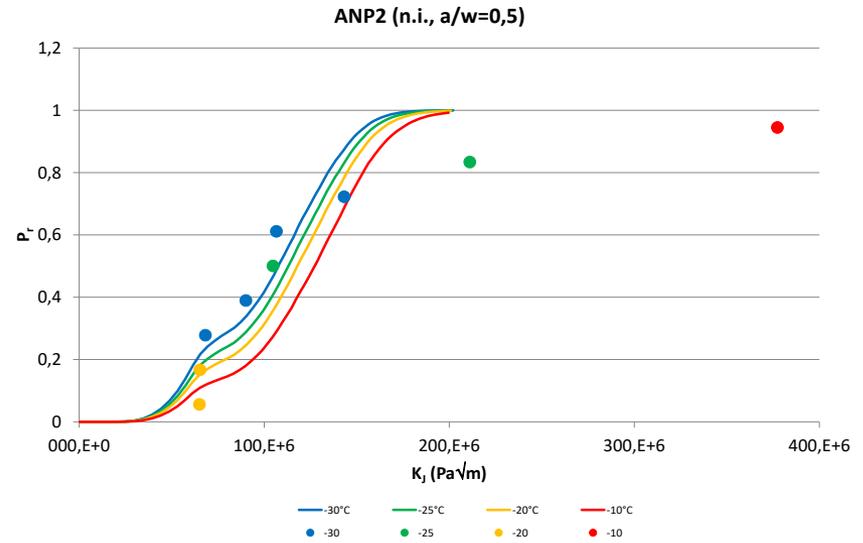


- ❑ MIBF model calibrated against the 3 cases for ANP-2, the calibrated values of γ_f were different, and higher than other steels (16.92 – 21.3 J/m²)
- ❑ Good results were obtained for both high constraint cases, including scatter.
- ❑ The irradiated low constraint case was more difficult to capture, MIBF under-predicted scatter and P_f saturated < 1.



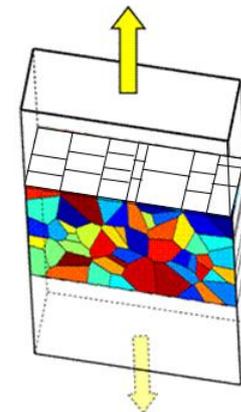
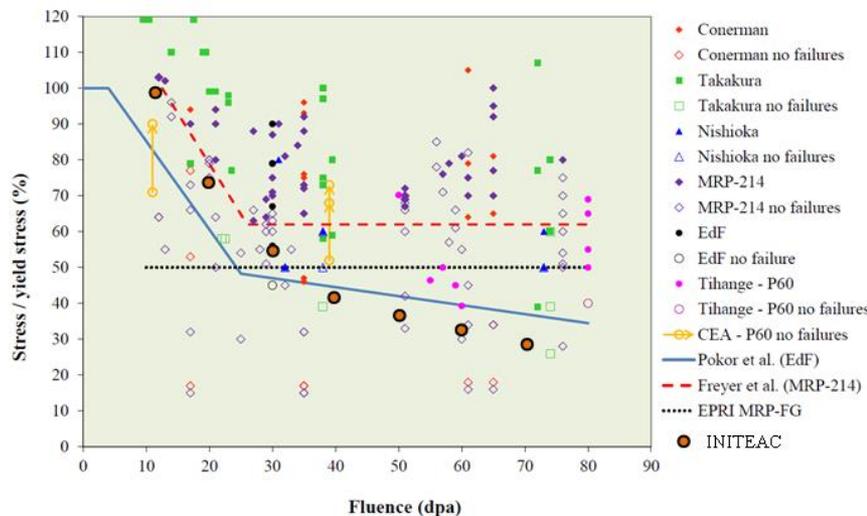
Application of MIBF to Weld (CEA)

- ❑ A $\gamma_f = 16.92 \text{ J/m}^2$ was applied across the 3 cases.
- ❑ Good results were obtained for high constraint non-irradiated and low constraint irradiated.
- ❑ The non-irradiated high constraint case predicted overly brittle behaviour.



INITEAC

- The INITAC model has been included to the platform.
- Further work is currently ongoing to include more recent understanding on physical processes relevant to IASCC;
 - A review of recent literature doesn't provide sufficient evidence to dramatically change the modelling process.
 - Review shows that some parameters can be better described and scatter/bounds improved.
 - *Review is being performed to examine influence of bounding inputs to the calculation to see which inputs are key to the calculation.*



- ❑ This presentation provides an overview of the final stage of the multi-scale process, i.e. available fracture models.
- ❑ The presentation also provides an overview of the ongoing activities within the SOTERIA Project related to fracture predictions.

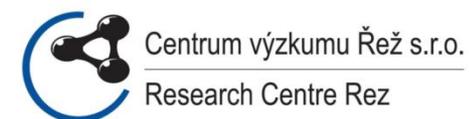
- ❑ The Cleavage Fracture LA models have considered:
 - Review effect of plasticity on cleavage fracture models,
 - Improve understanding of variation / outlying results,
 - Further experimental validation / comparison of models.

- ❑ The development for IASCC (INITEAC):
 - Focusing on understanding influence of scatter/bounds of input data and how this influences the prediction.
 - Review of new data useful to confirm approach adopted is still relevant.



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