MODELLING OF FISSION GAS RELEASE IN CHROMIA DOPED FUEL USING FEMAXI-6 COMPUTER CODE

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Abstract

A revised mechanistic model for fission gas diffusion in Chromia doped UO_2, based on the Cooper Variant A approach, has been implemented and evaluated in the FEMAXI-6 fuel performance code. The proposed formulation replaces the conventional effective diffusivity with a Cooper-corrected expression that retains the usual thermal, irradiation-enhanced, and fission-induced components, while accounting for the altered gas transport behavior of doped fuel. The model, built on the Booth intragranular diffusion solution and the Turnbull-type diffusivity framework widely used in engineering fuel performance analysis, introduces temperature-dependent corrections to better simulate fission gas mobility in doped UO_2. Its performance was assessed using experimental data, characterized by high linear power and significant fission gas release near the end of irradiation. The calculated peak fuel temperature, rod internal pressure, and cumulative fission gas release were compared with measurements. The model accurately reproduced fuel temperature and achieved reasonable agreement for rod internal pressure.

Keywords: *FEMAXI-6, Cooper model fission gas release, UO_2 doped fuel, intragranular diffusion*

Introduction

Doped UO_2 fuels, particularly chromia-doped and chromia/alumina-doped pellets, have drown considerable interest as near-term evolutionary accident-tolerant fuel (ATF) concepts because they preserve the conventional UO_2 - zirconium-alloy fuel system while introducing targeted microstructural modifications rather than a complete material substitution [1]. Current international assessments identify doped UO_2 as a higher-maturity advanced fuel technology, noting expected benefits such as increased grain size, improved fission-gas retention and potentially lower internal pressure and improved pellet-cladding interaction [1]. Recent review on literature suggests Cr-doped UO_2 as a promising near-term large-grain fuel concept, while also emphasizing that important questions remain regarding chromium incorporation, secondary phases, and the mechanistic link between dopant chemistry and in-reactor behaviour [2].

The interest in doped fuel arises from the fact that chromium additions modify more than grain size alone. Terricabras et al. showed that Cr-doping can produce average grain sizes exceeding 30 μm, with a maximum grain size of about 52 μm under the investigated fabrication conditions, while also affecting chromium retention, lattice incorporation, and thermal conductivity at higher dopant levels [2]. These findings provide a strong rationale for the explicit implementation of doped-fuel effects in engineering-scale fuel-performance codes. Cooper et al. developed an atomistically informed formulation for fission-gas diffusion in Cr_2O_3, showing that the impact of doping on intragranular Xe transport must be considered to assess fission-gas release under in-reactor conditions. More recently, Nicodemo et al. introduced an engineering model for chromium solubility and chromium-dependent fission-gas diffusivity in SCIANTIX [3], while de Lara et al. implemented dedicated Cr-doped fuel models, including a Cooper-based diffusion coefficient, in TRANSURANUS [4]. In this context, the implementation of a dopant-sensitive diffusion formulation in FEMAXI-6 is justified not as a minor numerical refinement, but as a necessary step toward a more physically consistent prediction of fuel temperature, rod internal pressure, and cumulative fission gas release in doped UO_2 fuel [4–6].

Diffusion and thermal conductivity models

To examine the sensitivity of the calculations to constitutive model selection, two fission gas diffusion models and two thermal conductivity models were considered. The diffusion behaviour of undoped UO_2 was described using the Turnbull formulation, in which the effective diffusivity is expressed as the sum of intrinsic, irradiation-enhanced, and athermal contributions. For Cr-doped fuel, the Cooper et al. correlation was implemented as a modified form of the Turnbull model, in which the intrinsic and irradiation-enhanced terms are corrected by temperature-dependent exponential factors, while the athermal contribution remains unchanged. In the present work, variant A of the Cooper model was adopted.

Thermal conductivity was represented using two alternative correlations. The first correlation was the MATPRO model, which describes UO_2 thermal conductivity by means of a piecewise temperature-dependent expression including density and porosity corrections. The second one was the revised Halden (Wiesenack) correlation, which accounts for the combined effects of temperature, porosity, and burnup. The calculations were therefore performed by combining the two diffusion models (Turnbull and Cooper) with the two thermal conductivity models (MATPRO and Halden), allowing the influence of both gas transport and heat conduction assumptions on the predicted fuel temperature, rod internal pressure, and fission gas release to be evaluated systematically.

Experimental database: Halden IFA 716

The experimental database used for validation includes data from the Halden IFA-716.1 irradiation program, which was designed to investigate the behaviour of Cr_2O_3-doped UO_2 fuels under in-pile conditions [6, 7]. The test was performed in the Halden reactor under HBWR conditions, using instrumented fuel rods equipped with plenum-pressure transducers and fuel centre thermos-couples, thereby providing integral information on the coupled evolution of thermal response, internal pressure, and fission gas release (FGR) [6, 7]. Publicly available benchmark descriptions indicate that the rig completed 12 irradiation cycles in IFA-716.1 and was subsequently reloaded for three additional cycles as IFA-716.2 [6, 7]. The test is thus particularly suitable for fuel-performance validation, since it combines in-pile thermal measurements with pressure-based assessment of gas release over an extended irradiation history [6, 7].

Rods 1 and 6 are the most frequently used validation cases for doped fuel, as both correspond to Framatome Cr_2 rods with documented fabrication characteristics and measured histories [6]. Reported benchmark conditions indicate average linear heat rates of approximately 24–30 kW/m (see Figure 1), while the online FGR evolution is commonly inferred from rod pressure [6, 7]. For rod 1, the pressure transducer failed before the end of irradiation, which limits the usable pressure- and FGR-history data for late times [7].

By contrast, rod 6 is often regarded as a more robust integral validation case because its end-of-life assessment includes puncture-based information after final unloading, providing a more reliable estimate of final gas release [7, 8]. Taken together, these features make IFA-716.1 a valuable database for assessing the predictive capability of fuel-performance models with respect to temperature, rod internal pressure, and cumulative FGR in chromia-doped UO_2 [6–8].

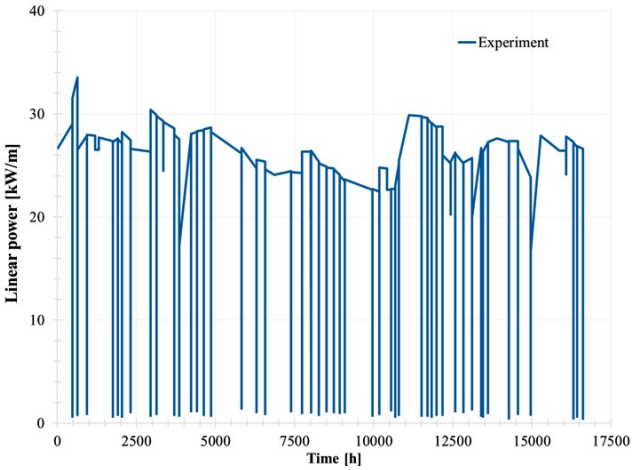


Fig. 1. Linear power history of IFA-716.1 Rod 6 as derived from the experimental data

Results and discussion

Figures 1 to 7 compares the measured and calculated thermal and gas-behaviour observables for IFA 716.1 rod 6 using the four model combinations. The figures show that the agreement in maximum fuel temperature is consistently good across all scenarios, with only slight deviations from the experimental value. The most significant differences are seen for rod pressure and cumulative FGR. The Cooper-based cases reproduce both observables with reasonable accuracy, whereas the Turnbull-based cases fail to predict measurable release and therefore substantially underestimate the integrated gas response. This comparison indicates that an acceptable prediction of peak temperature alone is not sufficient to guarantee correct gas-behaviour performance, since the latter depends mainly on the adopted diffusion formulation.

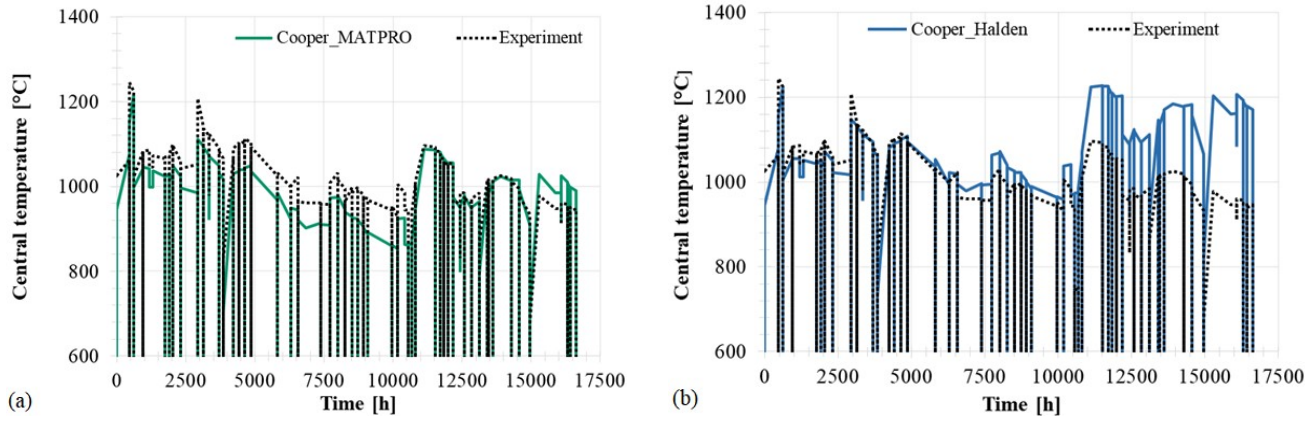


Fig. 2. Comparison of the experimentally measured maximum fuel centre temperature with FEMAXI-6 predictions obtained using the Cooper diffusion model and the MATPRO (a) and Halden (b) thermal conductivity models

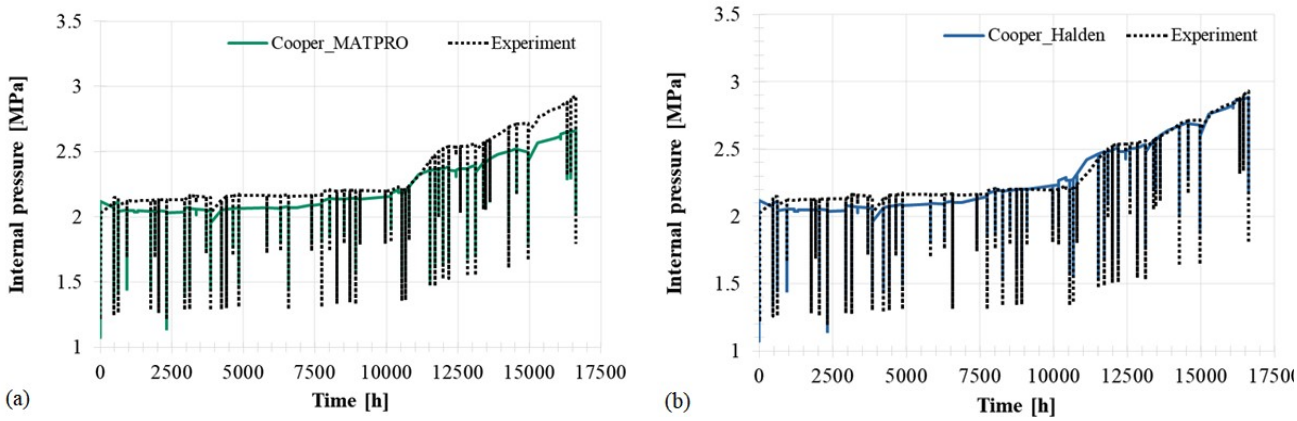


Fig. 3. Comparison of the experimentally measured maximum internal pressure with FEMAXI-6 predictions obtained using the Cooper diffusion model and the MATPRO (a) and Halden (b) thermal conductivity models

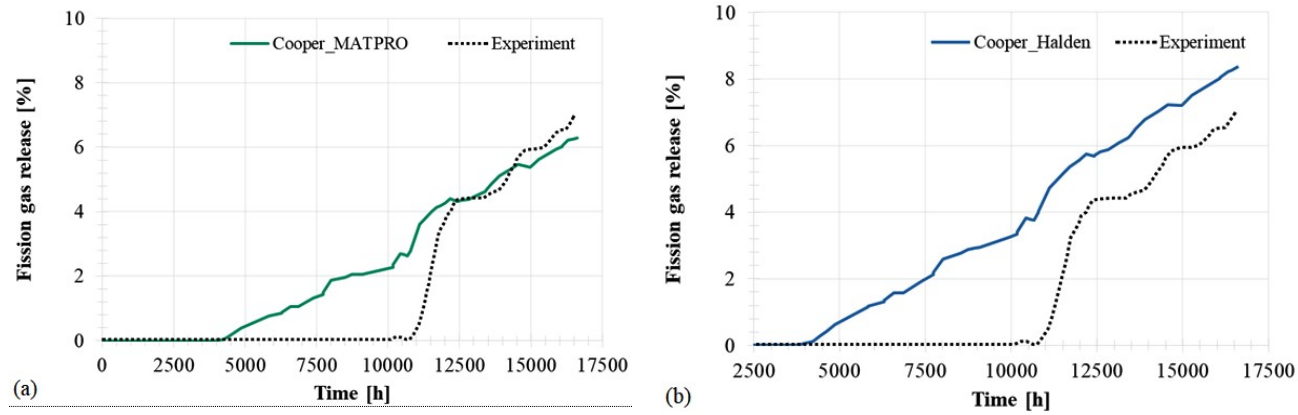


Fig. 4. Comparison of the experimentally measured cumulative fission gas release with FEMAXI-6 predictions obtained using the Cooper diffusion model and the MATPRO (a) and Halden (b) thermal conductivity models

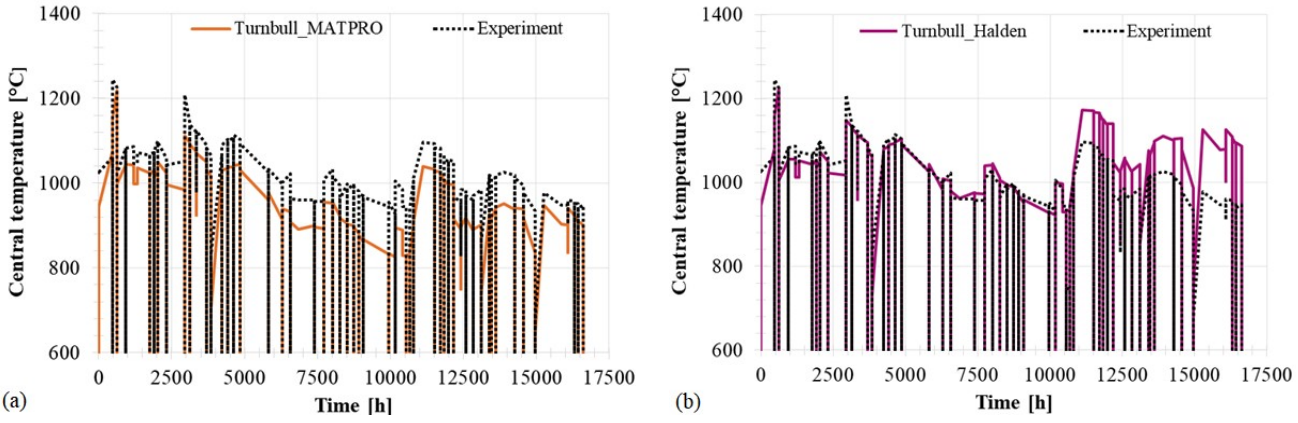


Fig. 5. Comparison of the experimentally measured maximum fuel centerline temperature with FEMAXI-6 predictions obtained using the Turnbull diffusion model and the MATPRO (a) and Halden (b) thermal conductivity models

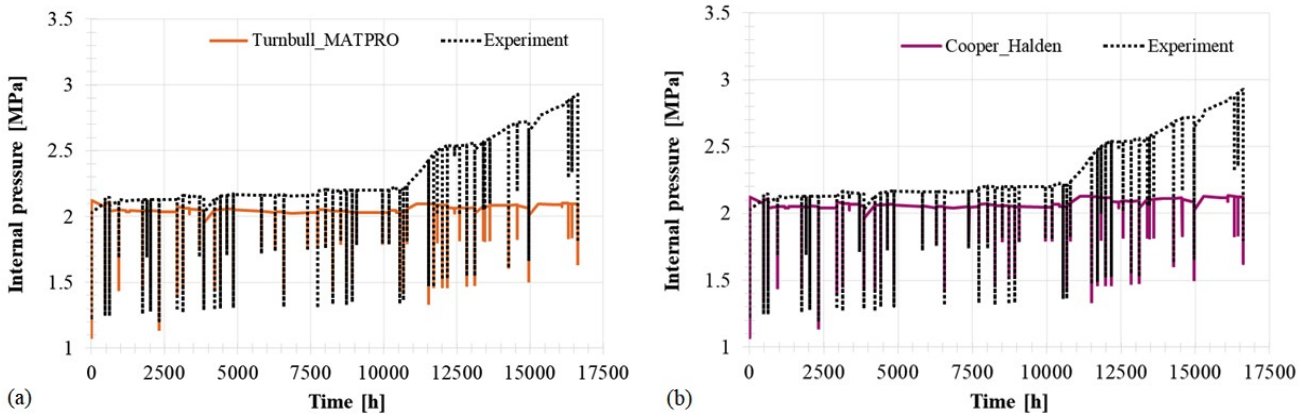


Fig. 6. Comparison of the experimentally measured maximum fuel internal pressure with FEMAXI-6 predictions obtained using the Turnbull diffusion model and the MATPRO (a) and Halden (b) thermal conductivity models

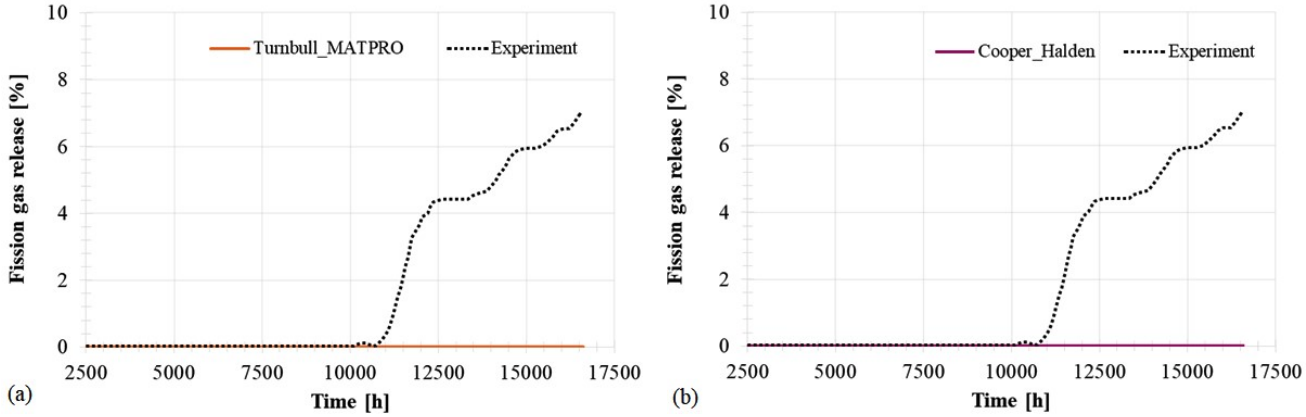


Fig. 7. Comparison of the experimentally measured cumulative fission gas release with FEMAXI-6 predictions obtained using the Turnbull diffusion model and the MATPRO (a) and Halden (b) thermal conductivity models

The comparison highlights an important methodological point: good thermal agreement does not automatically translate into good gas-behaviour agreement. Although all model combinations reproduce the peak fuel temperature within about 2%, only the Cooper-based diffusion model is able to generate a physically plausible level of gas release and the associated pressure increase. This suggests that the main limitation of the Turnbull-based cases is not the thermal field itself, but the insufficient activation of gas transport and release under the present irradiation conditions. At the same time, the difference between MATPRO and Halden affects the mean thermal level (see Table 2), which in turn modulates the magnitude of the predicted release. Cooper-MATPRO model responds slightly more conservatively than Cooper-Halden model, which raises both temperature and gas release, increasing pressure agreement but significantly overestimating FGR. Overall, the results support the conclusion that the diffusion model is the dominant factor governing predictive performance for internal pressure and FGR, whereas the conductivity model plays a secondary, indirect role via its influence on the temperature field.

Tables 1 and 2 summarize the experimental and computed values of maximum and mean fuel temperature, internal pressure, and cumulative fission gas release for rod 6. All four model combinations accurately reproduce the maximum fuel temperature, with ΔT_{max} ranging from 1.36% and 2.16%. In contrast, the selected conductivity model has a greater impact on the mean temperature. The MATPRO-based cases slightly underpredict the mean value (754.61 °C and 731.28 °C against 775.76 °C), whereas the Halden-based cases overpredict it (823.66 °C and 797.84 °C).

A much stronger discrimination is observed for internal pressure and fission gas release. The Cooper-based simulations yield non-zero FGR values (6.5–8.7%) and internal pressure levels (2.7–2.9 MPa) that are similar to the measured values (6.9% and 2.9 MPa), while the Turnbull-based cases predict zero FGR and lower internal pressure (2.1 MPa). These results indicate that, for the present study, the conductivity model mainly affects the thermal level, whereas the diffusion model controls the ability of the calculation to reproduce gas release and pressure build-up.

Table 1. Maximum and mean values obtained with FEMAXI-6 compared to experimental data

	Cooper-MATPRO						**Cooper-Halden**					
	T [°C]		P [MPa]		FGR [%]		T [°C]		P [MPa]		FGR [%]	
	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean
Measured	1245.5	775.76	2.9	2.12	6.9	3.8	1245.5	775.76	2.9	2.12	6.9	3.8
Calculated	1218.5	754.61	2.7	2.07	6.5	2.53	1228.5	823.66	2.9	2.14	8.7	3.4
	Turnbull-MATPRO						**Turnbull-Halden**					
	T [°C]		P [MPa]		FGR [%]		T [°C]		P [MPa]		FGR [%]	
	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean	Max.	Mean
Measured	1245.5	775.76	2.9	2.12	6.9	3.8	1245.5	775.76	2.9	2.12	6.9	3.8
Calculated	1218.5	731.28	2.1	1.92	0	0	1225.8	797.84	2.1	1.93	0	0

Table 2. Temperature related values for MATPRO and Halden thermal conductivity models

Parameter	**Cooper-MATPRO**	**Cooper-Halden**	**Turnbull-MATPRO**	**Turnbull-Halden**
$T_{exp,}max$ *[°C]*	1245.49	1245.49	1245.49	1245.49
$T_{calc,}max$ *[°C]*	1218.54	1228.51	1218.53	1225.81
ΔT_{max} *[%]*	2.16	1.36	2.16	1.58
$T_{exp,}mean$ *[°C]*	775.76	775.76	775.76	775.76
$T_{calc,}mean$ *[°C]*	754.61	823.66	731.28	797.84
ΔT_{mean} *[%]*	2.73	6.71	5.73	2.84
Mean Error [°C]	-21.1	47.9	-44.46	22.08
Normalized Mean Error [%]	-2.02	4.57	-4.24	2.11
Mean Absolute Error [°C]	40.38	64.9	22.08	42.06
Normalized Mean Absolute Error [%]	3.85	6.19	5.28	4.01

Conclusions

The comparative analysis reveals that all four model combinations reproduce thermal behavior with reasonable accuracy, as reflected by the small deviation in maximum fuel temperature from the experimental value. The inaccuracy in peak temperature remained less than about 2.2% in all cases, indicating that the general thermal response is adequately captured. Mean temperature shows greater differences, which are more sensitive to the selected thermal-conductivity correlation. The MATPRO-based calculations produce lower average temperatures, whereas the Halden-based calculations shift the thermal field upward, in some cases leading to overprediction.

The internal pressure and fission gas release results help to distinguish between selected models. The Cooper-based diffusion model produces non-zero FGR values and pressure levels close to those measured, demonstrating that it can reflect the gas transport and release processes active under the examined irradiation conditions. In contrast, the Turnbull-based calculations predict negligible gas release and significantly underestimate internal pressure, indicating that this formulation is insufficiently sensitive to the experimental release conditions. These results suggest that, in order to reproduce gas-behavior observables, selecting a diffusion model is more critical than the choice of a conductivity model.

Overall, the results support the use of the Cooper formulation as the more suitable diffusion model for the present case. The conductivity model primarily varies the temperature level and hence influences the quantitative amount of release; however, it does not alter the qualitative conclusion that the Cooper-based approach provides the best physically consistent agreement with the experimental data.

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