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# Optimization of signal processing obtained by $^1\text{H} \rightarrow ^{13}\text{C}$ polarization transfer to better characterize water structuring in biomaterials

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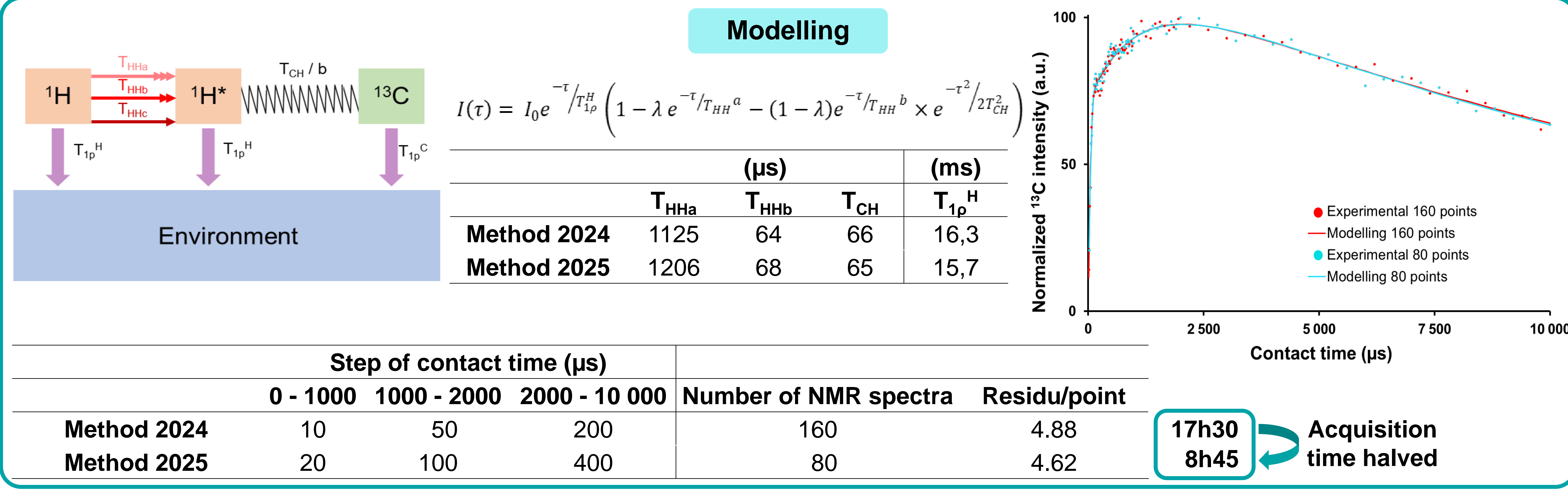
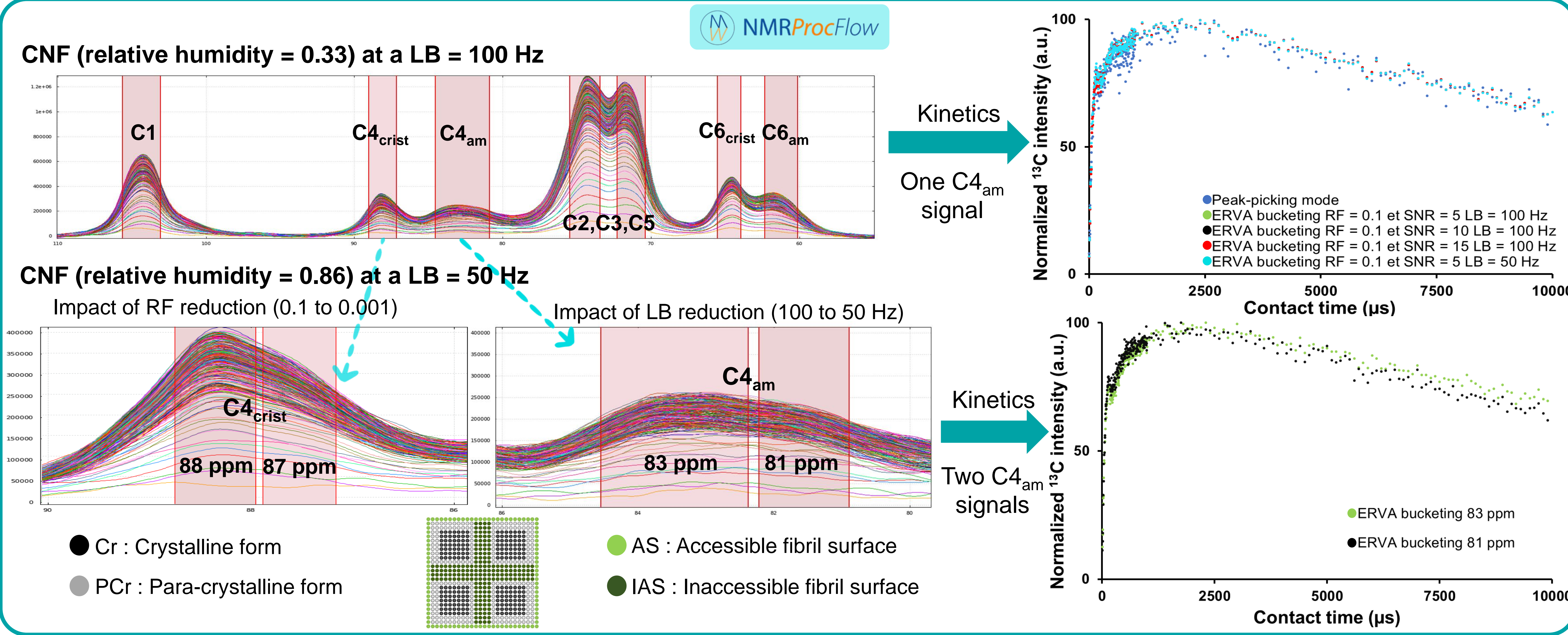
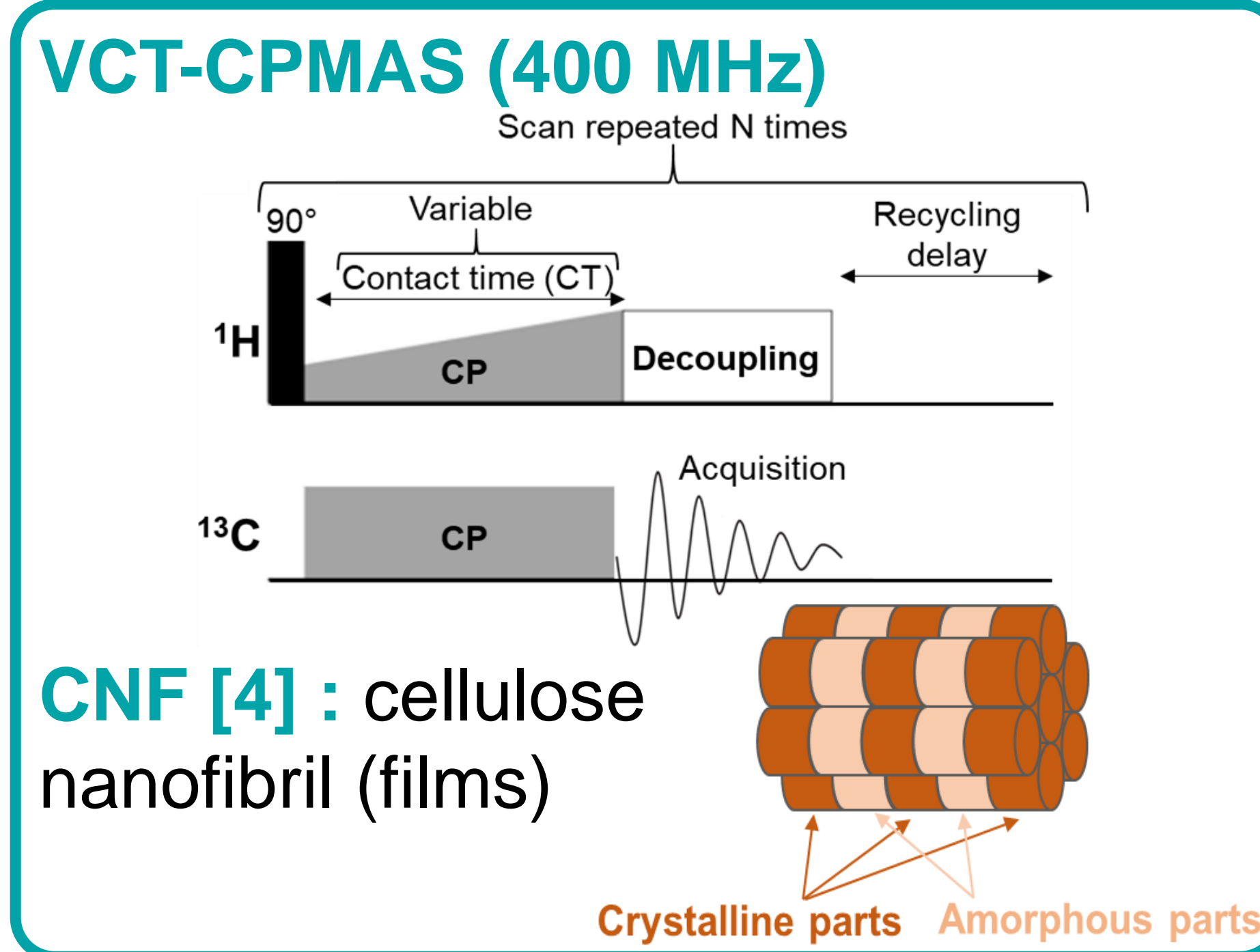
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**Background**  
As part of the ecological transition, biobased materials offer an alternative to petro-based plastics. **Solid-state  $^{13}\text{C}$  NMR** and **VCT-CPMAS** are used to study **water interactions** within these **biomaterials**. However, this experiment has a long acquisition time. An initial optimization of the protocols and **spectral processing** [1] has been carried out.  
→ Nevertheless these times remain restrictive, making further improvements necessary.

**Strategy**

- Adjustement of 2 parameters, Resolution factor (RF) and Signal-to-noise (SNR) to optimise the ERVA [2] **bucketing** conditions of NMRProcFlow software [3].
- Comparison with peak-picking using TopSpin
- Study of the influence of the apodization parameter (LB) on the kinetic profiles.
- Optimization of the number of NMR spectra required for the kinetics modelling and the residue analysis.



**Take Home messages**

- Processing time was reduced by 6 with NMRProcFlow using bucketing (batch mode), compared with peak-picking (sequential approach)
- Kinetics with less dispersion and access to potentially more information
- The results of the modelling have enabled us to halve the number of points required, resulting in an equivalent reduction in acquisition time

**References**  
[1] Falourd et al. *MethodsX* **2022** 9:101914. [2] Jacob et al. *Anal. Bioanal. Chem.* **2013** 405:5049. [3] Jacob et al. *Metabolomics* **2017** 13:36. [4] Falourd et al. *Data Brief* **2024**, 53:110106.