Molecular kinetics modeling in hemodialysis: on-line molecular monitoring and spectral analysis

Fernández, Elmer Andrés, Perazzo, Carlos Alberto, Valtuille, Rodolfo, Willshaw, Peter and Balzarini, Mónica (2007) *Molecular kinetics modeling in hemodialysis: on-line molecular monitoring and spectral analysis.* ASAIO Journal, 53 (5). pp. 582-586. ISSN 1058-2916

RESUMEN

The knowledge of the underlying molecular kinetics is a key point for the development of a dialysis treatment as well as for patient monitoring. In this work, we propose a kinetic inference method that is general enough to be used on different molecular types measured in the spent dialysate. It estimates the number and significance of the compartments involved in the overall process of dialysis by means of a spectral deconvolution technique, characterizing therefore the kinetic behavior of the patient. The method was applied to 52 patients to reveal the underlying kinetics from dialysate time-concentration profiles of urea, which has a well-known molecular kinetic. Three types of behaviors were found: one-compartmental (exponential decay Tau = 180 ± 61.64 minutes), bicompartmental (Tau1 = 24.96 ± 19.33 minutes, Tau2 = 222.32 ± 76.59 minutes), and tricompartmental (Tau1 = 23.03 ± 14.21 minutes; Tau2 = 85.75 ± 27.48 minutes; and Tau3 = 337 ± 85.52 minutes). In patients with bicompartmental kinetics, the Tau2 was related to the level of dialysis dose. The study concluded that spectral deconvolution technique can be considered a powerful tool for molecular kinetics inference that could be integrated in on-line molecular analysis devices. Furthermore, the method could be used in the analysis of poorly understood molecules as well as in new hemodialysis target biomarkers.

TIPO DE DOCUMENTO: Artículo

DOI: https://doi.org/10.1097/MAT.0b013e318145bb31

PALABRAS CLAVE: Biomarkers. Mathematical models. Molecular dynamics. Online systems. Patient monitoring.

TEMAS:	T Tecnología > TA Ingeniería de asistencia técnica (General). Ingeniería Civil (General)
UNIDAD ACADÉMICA:	Universidad Católica de Córdoba > Facultad de Ingeniería