Model-based comparison of batch and continuous preparative chromatography in the separation of rare earth elements

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Table S1: The calibrated model parameters values used in the simulations. A correlation was used for k_{kin}. Asterisks show values taken from Ojala et. al.[1]

Parameter	Value				Unit
q_{max}	700*				mol m^{-3} gel
β	2.3*				-
k_{kin}	$4.68 \cdot 10^{-7} \cdot \frac{1}{v}$				s^{-1}
	Nd	Sm	Eu	Gd	
H^o	0.27*	0.59*	0.86*	1.13*	$(\text{mol m}^{-3})^{\beta}$

Table S2: Objective values [Y, Sp] for the Y-Sp optimizations. Three operating points are chosen for $w = 0$ (maximum yield), $w = 1$ (maximum solvent productivity) and $Y_{90\%}$ (90 % yield)

	$w = 0$	$Y_{90\%}$	$w = 1$
Batch	[98.8, 0.026]	[90.0, 0.16]	[51.2, 0.29]
MCSGP	[99.5, 0.14]	[90.0, 0.30]	[60.3, 0.40]

Table S3: Objective values [Y, Pr] for the Y-Pr optimizations. Three operating points are chosen for $w = 0$ (maximum yield), $w = 1$ (maximum productivity) and $Y_{90\%}$ (90 % yield)

	$w = 0$	$Y_{90\%}$	$w = 1$
Batch	[99.0, 0.030]	[90.0, 0.27]	[50.5, 0.51]
MCSGP	[100.0, 0.11]	[90.0, 0.39]	[61.7, 0.52]

Table S4: The individual yields and productivities for $Y_{90\%}$ (the closest Pareto point over 90 %) in the Y-Pr optimizations for batch and MCSGP. Y are the weighted sum of Y_{Sm}, Y_{Eu}, Y_{Gd} and Pr are the weighted sum of $\mathrm{Pr}_{\mathrm{Sm}}$,$\mathrm{Pr}_{\mathrm{Eu}}$, $\mathrm{Pr}_{\mathrm{Gd}}$.

	Y	Y_{Sm}	Y_{Eu}	Y_{Gd}	Pr	$\mathrm{Pr}_{\mathrm{Sm}}$	$\mathrm{Pr}_{\mathrm{Eu}}$	$\mathrm{Pr}_{\mathrm{Gd}}$
Batch	90.4	100.0	86.3	93.1	0.27	0.83	0.072	0.078
MCSGP	91.1	95.6	88.6	96.0	0.38	1.19	0.095	0.12

References

(1) Ojala, F.; Max-Hansen, M.; Kifle, D.; Borg, N.; Nilsson, B. Modelling and Optimisation of Preparative Chromatographic Purification of Europium. *J. Chromatogr. A* **2012**, *1220*, 21.