MODELING OF SOLUBILITY OF 1-AMINOANTHRAQUINONE AND 1 - NITROANTHRAQUINONE IN SC-CO_2 USING ARTIFICIAL NEURAL NETWORK (ANN) AND PARTICLE SWARM OPTIMIZATION ALGORITHM (PSO)

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ABSTRACT

In this work, a hybrid method based on ANN and PSO algorithm [1] is applied to develop and validate a model that can predict with precision solubility of 1-aminoanthraquinone and 1 -nitroanthraquinone in supercritical carbon dioxide [2]. The PSO [3] was used for two purposes: replacing the standard back propagation in training the ANN and optimizing the process. Statistical analysis of the predictability of the optimized neural network model shows excellent agreement with experimental data (coefficient of correlation equal to 0.997). Furthermore, the comparison in terms of average relative deviation (AARD%) between, the predicted results for the whole temperature and pressure range shows that the optimized ANN-PSO model can predict far better the solubility of two solid drugs than the semi-empirical models and cubic equations of state.

Keywords: Phase Equilibria, Solid drugs, Solubility, Artificial Neural Networks, Particle Swarm Optimization, Modeling, supercritical carbon dioxide

Table 1: Structure of the optimized ANN-PSO model

	Input Layer	Hidden Layer		Output Layer		Training Algorithm
	Nb of neurons	Nb of neurons	Activation Function	Nb of neurons	Activation Function	TRAINSPO
MLP	4	4	TANSIG	1	Purline	

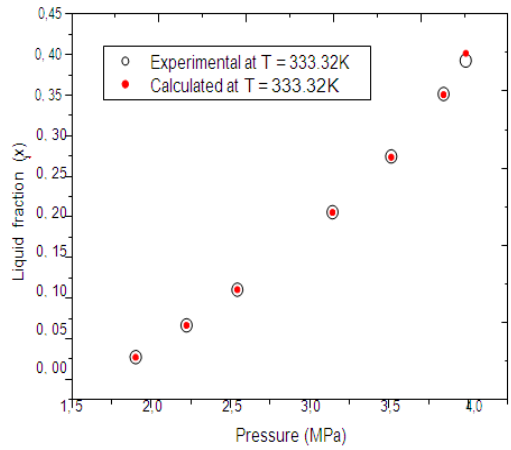

Figure 2: graphical comparison between experimental and predicted solubility by ANN-PSO model at 333.32 K.

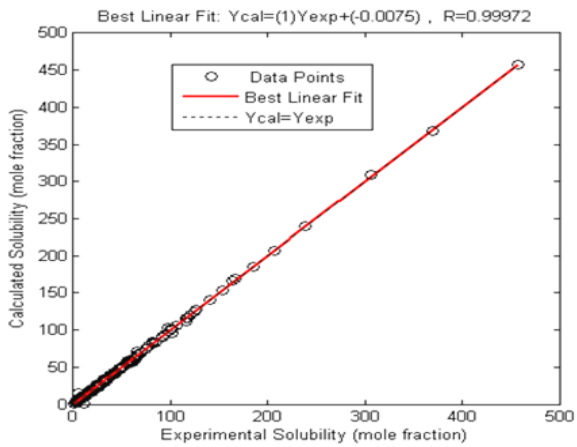

Figure 3 Comparison between experimental solubility and predicted by ANN-PSO model in terms of coefficient of regression.

REFERENCES

[1] J. Bourquin, H. Schmidli H, P. Hoogvest and H. Leuenberger, Basic concept of artificial neural networks (ANN) modelling in the application of pharmaceutical development, Pharm. Dev. Technol. 2, 95, 1997.

[2] Kazuhiro Tamura, Ratna Surya Alwi, Tatsuro Tanaka, Keisuke Shimizu, Solubility of 1-aminoanthraquinone and 1-nitroanthraquinone in supercritical carbon dioxide, J. Chem. Thermodynamics, 104, pp 162–168, 2017.

[3] Battiti R, Reactive search: towards self-tuning heuristic In: Modern heuristic search methods, Wiley, pp 61–83, 1996.