

Title (en)

METHOD FOR CONSTRUCTING A MODEL SIMULATING A CHEMICAL REACTION

Title (de)

VERFAHREN ZUR KONSTRUKTION EINES EINE CHEMISCHE REAKTION SIMULIERENDEN MODELLS

Title (fr)

PROCEDE DE CONSTRUCTION D'UN MODELE DE SIMULATION D'UNE REACTION CHIMIQUE

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Application

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Abstract (en)

[origin: WO2022233602A1] The present invention relates to a method for constructing a model (MSI) simulating at least one chemical reaction, which constructs an intermediate model by means of an artificial neural network (RNA) and of a training database (BAP), and that then constructs the simulating model by adding an additional mass-conservation layer (RNC) to the artificial neural network (RNA). Furthermore, the invention relates to a method for simulating (SIM) a chemical reaction that implements the constructed simulating model (MSI).

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