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A simple approach to improve the robustness of equation-oriented simulators: Multilinear look-up table interpolators



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ABSTRACT

Equation-oriented simulators have some advantages over the modular sequential ones, but improvements are still necessary to deal with nonlinearities, while preserving the robustness of the solver. Linear approximations and/or surrogate models can be used in place of nonlinear models, but the loss of predictive accuracy may be a drawback. An alternative to circumvent this problem is the use of grid-based look-up tables for interpolating responses from rigorous models. This methodology was integrated in an equation-oriented simulator (EMSO). A case study involving the production of bioethanol from sugarcane is used to demonstrate the robustness of this approach. Look-up tables replaced the models of two distillation column trains and of the cellulose hydrolysis reactor. These models were included into the global process and an optimization problem aiming at the maximum production of ethanol was successfully solved by a PSO algorithm varying the solid mass fraction in the hydrolysis reactor.

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1. Introduction

Equation-oriented process simulators solve the system of equations simultaneously. Although useful when the number of recycle streams in the process is large, this approach prevents the implementation of strategies for circumventing local convergence problems (i.e., including ad hoc algorithms within the models of specific process units, the “modules” of the sequential modular simulators). According to Morton (2003), processes with awkward nonlinearity and high recycle complexity should be solved by equation-oriented simulators, provided their robustness undergoes some improvements. Nevertheless, while such generically robust solver is not available, some strategies can be developed to

circumvent this bottleneck. As a general case, these strategies rely on simplifications of the models that constitute the chemical plant. However, these simplifications generally imply loss of accuracy and operational flexibility (Morton, 2003).

Here, an alternative approach is presented: using grid-based look-up tables to interpolate the results of previous offline simulations, for the process unit models whose nonlinearity was hindering the convergence of the simulations of the overall industrial plant. With this simple strategy, the accuracy of the simplified model (the interpolator) can be tuned, while still requiring low computational power (Nelles, 2001). As a proof of concept, an integrated first and second generation ethanol biorefinery was modeled, using both sugarcane and sugarcane leaves as feedstock. Two process sections, chosen for their characteristically nonlinear behavior, were used for testing the methodology: the distillation columns trains, which were simulated in steady-state, and the enzymatic hydrolysis reactor, which was simulated dynamically, with the results at the end of the batch run being considered in the global process simulations. In both cases, results obtained with this methodology were compared to the ones generated by the original phenomenological models. The look-up table interpolators were then coupled

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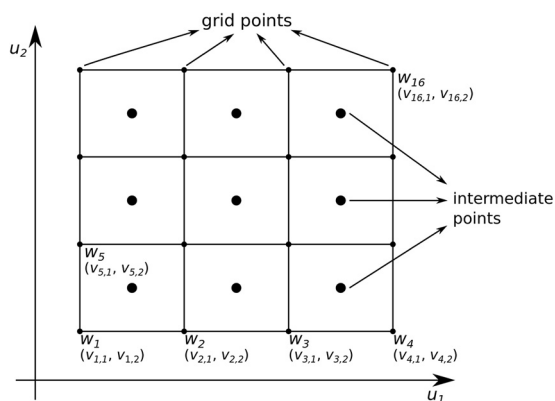


Fig. 1. Example of a two-dimensional grid with the intermediate points used to test the grid accuracy. w is the output variable (a scalar) and v the input variables vector (here, two-dimensional) at the grid nodes. u is a new input vector to be interpolated.

to the global process flowsheet, in order to evaluate the robustness of the approach.

2. Methodology

2.1. Simulator

The simulator EMSOTM (Environment for Modeling Simulation and Optimization), used in this work, is equation-oriented. This simulator has an internal object-oriented modeling language that allows insertion of new models into its internal library. Moreover, it is possible to add plug-ins for running calculations which are not suitable for the equation-oriented approach; and new solvers may be linked as dynamic libraries as well (Soares and Secchi, 2003).

2.2. Grid-based look-up tables

Grid based look-up tables consist of a set of data points positioned in a multi-dimensional grid. The scalar values w_i in the grid are the estimates (or the actual values) of the nonlinear function for a given vector of n input variables $v_{i,k}$, (v is a matrix where each column corresponds to a point in the grid and each row to one element of the input variables vector, Vogt et al., 2004). Fig. 1 illustrates the two-dimensional case ($n=2$). The output of the interpolator is determined by considering the smallest n -cube or n -parallelepiped (C) defined by the grid points v_i , columns of the matrix v which enclose a new input vector u (i.e., the input variables whose corresponding model output, \hat{y} , is required to be calculated). The interpolated output (\hat{y} , a scalar) is a weighted average of the output values (w_i) at each vertex of C (whose coordinates are given by the i -column of v , v_i), with weights Φ_i , Equation (1). These weights (Φ_i) are the ratios between the volume of each n -cube whose longer n -diagonal is defined by u and the vertex v_j of C that is opposed to v_i (i.e. the coordinates v_i and v_j define a longer diagonal of C), divided by the total volume of C (Nelles, 2001):

$$\hat{y} = \sum_{i=1}^M w_i \Phi_i(u, v) \quad (1)$$

According to this definition, the closer each column of v (v_i , corresponding to a set of input variables) is from u , the higher will be its weight. Eq. (1) is a basis function formulation for \hat{y} . Hence, the value of Φ_i is actually defined for the whole interpolation region (defined by the M interpolation points), being zero for all n -cubes'

Table 1

Input variables and process specifications for the simulations of the hydrous ethanol distillation columns train.

	Description	Value
Input variables	Input stream temperature (K)	348.15–378.15
	Input stream ethanol mass fraction	0.065–0.105
Process specifications	Ethanol mass fraction in hydrous ethanol	0.935
	Ethanol mass fraction in vinasse	0.002
	Ethanol mass fraction in Phlegmasse	0.002
	Ethanol recovered in the vapor phlegm stream	76%

vertices except for the ones of the n -cube C , which encloses u (Eq. (2)), with M being obtained by Eq. (3).

$$\phi_i(u, v) = \begin{cases} \frac{\prod_{k=1}^n |u_k - v_{j,k}|}{\prod_{k=1}^n |v_{i,k} - v_{j,k}|}, & \text{when } i \text{ is a vertex of } C \\ 0, & \text{when } i \text{ is not a vertex of } C \end{cases} \quad (2)$$

$$M = \prod_{k=1}^n M_k \quad (3)$$

where M_k is the number of points in the grid for the input variable k and n is the number of input variables.

Many applications of look-up tables implement uniformly distributed input variables. This choice allows fast access to the neighboring points (C) by address computation. However, it also restricts the flexibility of the look-up table since the spacing cannot be adjusted to increase accuracy where it is needed (Nelles, 2001). In the present study, only look-up tables with uniformly distributed grids were implemented. Accuracy evaluations were performed to determine the minimum number of points in the grid for each variable. A maximum relative error of 5% was considered in this analysis for absolute values greater than one, while the absolute error (with a maximum of 0.05) was considered for absolute values smaller than one. Intermediate points in the center of the most refined grid were used as test for the accuracy of the grids (Fig. 1). The interpolated points for each look-up table were compared with the “exact” values (provided by phenomenological models).

2.3. Distillation columns

Distillation columns for bioethanol purification were configured according to Dias (2008). In a conventional configuration, two columns are used and saturated vapor of hydrous ethanol is obtained with ethanol mass fraction of 0.935 (w/w).

Column trains were simulated in ASPEN PLUS[®] using RADFRAC model. The liquid phase was described by Wilson model, while the vapor phase was assumed to be ideal. It was considered that the wine was composed only by ethanol and water. Temperature and ethanol mass fraction of the feed stream were elected as input variables for the look-up tables (Table 1). The output variables were the heat duties of columns' reboilers and condensers, the molar fraction of ethanol at the top of the first column, the molar flowrates of first column bottom (vinasse), first column top (second grade ethanol), second column bottom (flegmasse) and second column top (hydrous ethanol). Except for the molar fraction of ethanol at the top of the first column, all output variables were divided by the mass flowrate of the first column feed in order to obtain an intensive value, independent of the inlet flowrate. Three look-up tables with 15, 45 and 153 points and constant intervals were generated.

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