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PROCEDURA IZRAČUNAVANJA VISKOZNOSTI NEZASIĆENIH ESTARA PRIMENOM PROŠIRENOG MODELA ČVRSTE SFERE

THE PROCEDURE FOR CALCULATING THE VISCOSITY OF UNSATURATED ESTERS APPLYING THE EXTENDED HARD-SPHERE MODEL

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Estri su prirodne supstance prisutne u raznim biljnim vrstama kojima daju svoj karakterističan ukus i miris. Oni su važna komponenta smeše estara masnih kiselina prisutnih u biodizelu i zbog ove činjenice i višestrukih industrijskih primena, poznavanje viskoznosti estara je suštinski preduslov za dobar dizajn procesa i optimalan rad.

Cilj je bio da se obezbedi model sa jakom fizičkom osnovom koji će omogućiti tačna predskazivanja viskoznosti tečnih zasićenih i nezasićenih metil i etil estara. U prvom koraku je formirana baza podataka iz pregleda literature za zasićene metil i etil estre do metil tetrakosanoata i etil eikosanoata. Prošireni model čvrste sfere, koji ima svoju osnovu u kinetičkoj teoriji i molekularnom opisu fluida, primenjen je za određivanje efektivnih parametara V_0 i R_η korelisanjem podataka za viskoznost. Ovi parametri se tretiraju kao funkcija temperature i molarne mase i određena je jedinstvena zavisnost za metil i etil estre. Podaci za viskoznost su predstavljeni sa AAD od 1,5% i 1,8% za zasićene metil i etil estre, redom.

Prikazana analiza se ne može izvršiti za nezasićene estre zbog nedostatka dostupnih podataka. Naš pristup je bio da koristimo koncept 'efektivne M_w', gde se M_w i R_η koriste za nezasićeni estar, zajedno sa V_0 zasićenih metil ili etil estara, da bismo korelisali ograničeni broj podataka za viskoznost nezasićenih estara. Ovo je ekvivalentno mapiranju V_0 nezasićenog estra sa onima zasićenih, koristeći M_w kao efektivni parametar. Preliminarni proračuni, verifikovani na osnovu veoma male baze podataka, pokazuju da predloženi model ima potencijal. Rezultati dobijeni za nezasićene metil i etil estre oleat, linoleat i linolenat pokazuju odstupanja od 0,8% i 2,0% od eksperimentalnih podataka, redom.

Ključne reči: *etil oleat; etil linoleat; etil linolenat; prošireni model čvrste sfere; viskoznost*

Esters are naturally occurring chemicals present in various plant species to which they give their characteristic taste and smell. They are an important component of mixtures of fatty acid esters present in biodiesel and due to this fact and multiple industrial applications, knowledge of the viscosity of esters is an essential pre-requisite for good process design and optimal operations.

The aim was to provide a model with a strong physical basis that will allow accurate predictions of viscosity of the liquid saturated and unsaturated methyl and ethyl esters. In the first step data

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set was formed from literature survey for saturated methyl and ethyl esters up to methyl tetracosanoate and ethyl eicosanoate. The Extended Hard-Sphere Model, that has its basis in kinetic theory and the molecular description of the fluid, was applied to determine effective parameters V_0 and R_η by fitting to viscosity data. These parameters are treated as a function of temperature and molar mass and the unique dependence is determined for methyl and ethyl esters. The viscosity data were represented with the AAD of 1.5% and 1.8% for saturated methyl and ethyl esters, respectively.

The presented analysis cannot be performed for unsaturated esters due to the lack of available data. Our approach was to use the concept of 'effective M_w', where M_w and R_η are used of unsaturated ester, together with V_0 of saturated methyl or ethyl esters, to correlate the limited viscosity data of the unsaturated esters. This is equivalent to mapping V_0 of unsaturated ester to those of the saturated ones, using M_w as the effective parameter. Preliminary calculations, verified against a very small data set, show that the proposed model has potential. Results obtained for the unsaturated methyl and ethyl esters oleate, linoleate and linolenate show deviations of 0.8% and 2.0% from experimental data, respectively.

Key words: *ethyl oleate; ethyl linoleate; ethyl linolenate; extended hard-sphere model; viscosity*