





# Improved SPC force field of water based on the dielectric constant: SPC/ $\epsilon$

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## Abstract

In a recent work, Fuentes and Alejandro (2014) found that for TIP4P models there is a dipole moment of minimum density at 240 K and that the Lennard-Jones parameters can be adjusted to match the experimental dielectric constant at 300 K and the temperature of maximum density, respectively. The same procedure is used in this work to re-parameterize the simple point charge (SPC) model keeping the original geometry. The new model fails to reproduce the experimental self-diffusion coefficient and shear viscosity but improves the results at different temperatures and pressures of dielectric constant, isothermal compressibility, thermal expansion coefficient, surface tension, coexisting densities at the liquid–vapor interface, equation of state of ice Ih and equation of state of liquids at high pressures. A second model that reproduces the dielectric constant, self-diffusion coefficient and shear viscosity is proposed but the temperature of maximum density is 250 K, compared with the experimental value of 277 K. Both models improve the SPC/E results for almost all properties. The TIP3P model was also analyzed but the liquid density at 240 K always increases and a minimum in the dipole moment was not found. It is not possible to adjust for that model the charge distribution and short range interaction parameters to reproduce at the same time the target properties.

## Introduction

The non-polarizable force fields of water have been reviewed in several works [1], [2], [3]. Vega et al. [3] in 2011 established that the best model to reproduce more experimental properties of water was the