

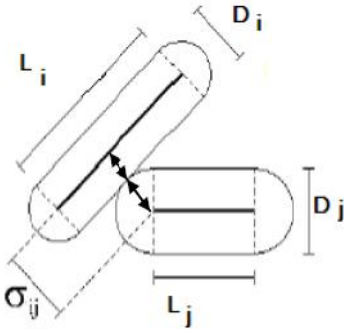


SDI FINAL EVALUATION FORM 1.1

PART 1:

Journal Name:	Physical Review & Research International
Manuscript Number:	MS: 2012 PRRI 2642
Title of the Manuscript:	Direct Correlation Function of Hard Molecular Fluid

PART 2:

FINAL EVALUATOR'S comments on revised paper (if any)	Authors' response to final evaluator's comments
<p>The response of authors is not convenient. Eqs. 21and 22 are not closest approach of SC.</p>	<p>Dear Dr. Avazpour</p> <p>Thank you so much for your advice. DCF of hard SC fluids were obtained by using two new different methods of closest approach. As you know, in molecular liquid theory calculating the closest approach between two molecules is very important. In order to calculate the DCF of the fluid it is necessary to calculate the closet approach between the molecules.</p> <p>We use two new different methods for calculating the closest approach. In one of them we used the finite element method. This method that we propose is the numerical method. The shortest distance between SCs is just the shortest distance between rods, σ_{ij} (that are shown with L_i and L_j , the main axis of the SCs (cylinders axis))minus the half diameter of the each SC($\frac{D_i}{2} + \frac{D_j}{2}$).</p>  <p>Therefore by using finite element method the closest approach of two rods is calculated first. In this method, the main axis of the SCs (cylinders axis) are divided into equal parts. Eqs. 21 and 22 describe the coordinate of the beginning and end points of the main axis of the cylinder, and the coordinate of the ith node of one cylinder axis, respectively. These equations include the distance between the center and orientation of each molecule ($\mathcal{Q}_i = (\theta_i, \varphi_i), \vec{r}_{i2}$). The main axis of the other cylinder is divided into <i>m</i> equal parts similarly. In second step, the distances between the pairs of points listed from each cylinder which is the combination of 2 from <i>m+n</i> are calculated. The minimum value from the calculated distances is chosen. It is the shortest distance between the main axis of the SCs (cylinders axis).</p> <p>For example n=3 and m=4. For 12 states that are shown in figure, the distance between the points should be calculated. Whatever the number of nodes is greater, calculations would be more accurate.</p>



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These steps describe in lines 139-158.

In the other method we use a fast algorithm proposed by Vega and Lago. They actually applied their method for calculating the closest approach between two rods and we extend this to find the closest approach between two SCs.

According to the results shown in the Table 1, for the aspect ratio, $L/D=5.0$, these methods are in good agreement.

These methods are more general and can also be used for the mixtures.

All programs are written in MATLAB.

I should mention that if the finite element method can be used, the problems are calculated much faster and more accurate than other methods.