Dynamic simulation of shear thickening in concentrated colloidal suspensions

FM 10120.

1 Supplement to Dratler, Schowalter, and Hoffman

Expressions for the resistance tensors used in equation (11) of Dratler, Schowalter, and Hoffman are given below. These expressions are based on formulas given in Kim & Karrila (1991). The A tensors can be expressed as

$$A_{ij}^{10} = X_A^{12}(h_1)d_{1i}d_{1j} + Y_A^{12}(h_1)\left(\delta_{ij} - d_{1i}d_{1j}\right) , \tag{A.1}$$

$$\begin{aligned} A_{ij}^{11} &= X_A^{11}(h_2)d_{2i}d_{2j} + Y_A^{11}(h_2)\left(\delta_{ij} - d_{2i}d_{2j}\right) \\ &+ X_A^{11}(h_1)d_{1i}d_{1j} + Y_A^{11}(h_1)\left(\delta_{ij} - d_{1i}d_{1j}\right) + \delta_{ij} , \end{aligned} \tag{A.2}$$

$$A_{ij}^{12} = X_A^{12}(h_2)d_{2i}d_{2j} + Y_A^{12}(h_2)\left(\delta_{ij} - d_{2i}d_{2j}\right) , \tag{A.3}$$

$$A_{ij}^{21} = A_{ji}^{12} , \tag{A.4}$$

$$\begin{aligned} A_{ij}^{22} &= X_A^{11}(h_2)d_{2i}d_{2j} + Y_A^{11}(h_2)\left(\delta_{ij} - d_{2i}d_{2j}\right) \\ &+ X_A^{11}(h_3)d_{3i}d_{3j} + Y_A^{11}(h_3)\left(\delta_{ij} - d_{3i}d_{3j}\right) + \delta_{ij} , \end{aligned} \tag{A.5}$$

$$A_{ij}^{23} = X_A^{12}(h_3)d_{3i}d_{3j} + Y_A^{12}(h_3)\left(\delta_{ij} - d_{3i}d_{3j}\right) , \tag{A.6}$$

for $i = 1, 2$ and $j = 1, 2$. The quantity δ_{ij} is the Kronecker delta. The B tensors can be expressed as

$$B_{ij}^{10} = -Y_B^{12}(h_1)\epsilon_{ijk}d_{1k} , \tag{A.7}$$

$$B_{ij}^{11} = Y_B^{11}(h_2)\epsilon_{ijk}d_{2k} - Y_B^{11}(h_1)\epsilon_{ijk}d_{1k} , \tag{A.8}$$

$$B_{ij}^{12} = Y_B^{12}(h_2)\epsilon_{ijk}d_{2k} , \tag{A.9}$$

$$B_{ij}^{21} = -B_{ij}^{12} , \tag{A.10}$$

$$B_{ij}^{22} = -Y_B^{11}(h_2)\epsilon_{ijk}d_{2k} + Y_B^{11}(h_3)\epsilon_{ijk}d_{3k} , \tag{A.11}$$

$$B_{ij}^{23} = Y_B^{12}(h_3)\epsilon_{ijk}d_{3k} , \tag{A.12}$$

for $i = 3$ and $j = 1, 2$. The quantity ϵ_{ijk} is the alternating tensor. The $\tilde{B}$ tensors can be expressed as

$$\tilde{B}_{ij}^{10} = -B_{ji}^{10} , \tag{A.13}$$

$$\tilde{B}_{ij}^{11} = B_{ji}^{11} , \tag{A.14}$$

$$\tilde{B}_{ij}^{12} = B_{ji}^{21} , \tag{A.15}$$

$$\tilde{B}_{ij}^{21} = B_{ji}^{12} , \quad (A.16)$$
$$\tilde{B}_{ij}^{22} = B_{ji}^{22} , \quad (A.17)$$
$$\tilde{B}_{ij}^{23} = -B_{ji}^{23} , \quad (A.18)$$

for $i = 1, 2$ and $j = 3$. The C tensors can be expressed as

$$C_{33}^{10} = Y_C^{12}(h_1) , \quad (A.19)$$
$$C_{33}^{11} = Y_C^{11}(h_1) + Y_C^{11}(h_2) + \frac{4}{3} , \quad (A.20)$$
$$C_{33}^{12} = Y_C^{12}(h_2) , \quad (A.21)$$
$$C_{33}^{21} = C_{33}^{12} , \quad (A.22)$$
$$C_{33}^{22} = Y_C^{11}(h_2) + Y_C^{11}(h_3) + \frac{4}{3} , \quad (A.23)$$
$$C_{33}^{23} = Y_C^{12}(h_3) . \quad (A.24)$$

The $\tilde{G}$ tensors can be expressed as

$$\begin{aligned}
\tilde{G}_{ijk}^{10} &= X_G^{12}(h_1)\left(d_{1j}d_{1k} - 1/3\delta_{jk}\right)d_{1i} \\
&+ Y_G^{12}(h_1)\left(d_{1j}\delta_{ki} + d_{1k}\delta_{ji} - 2d_{1i}d_{1j}d_{1k}\right) , && (A.25) \\
\tilde{G}_{ijk}^{11} &= X_G^{11}(h_2)\left(d_{2j}d_{2k} - 1/3\delta_{jk}\right)d_{2i} \\
&+ Y_G^{11}(h_2)\left(d_{2j}\delta_{ki} + d_{2k}\delta_{ji} - 2d_{2i}d_{2j}d_{2k}\right) \\
&- X_G^{11}(h_1)\left(d_{1j}d_{1k} - 1/3\delta_{jk}\right)d_{1i} \\
&- Y_G^{11}(h_1)\left(d_{1j}\delta_{ki} + d_{1k}\delta_{ji} - 2d_{1i}d_{1j}d_{1k}\right) , && (A.26) \\
\tilde{G}_{ijk}^{12} &= -X_G^{12}(h_2)\left(d_{2j}d_{2k} - 1/3\delta_{jk}\right)d_{2i} \\
&- Y_G^{12}(h_2)\left(d_{2j}\delta_{ki} + d_{2k}\delta_{ji} - 2d_{2i}d_{2j}d_{2k}\right) , && (A.27) \\
\tilde{G}_{ijk}^{21} &= -\tilde{G}_{ijk}^{12} , && (A.28) \\
\tilde{G}_{ijk}^{22} &= -X_G^{11}(h_2)\left(d_{2j}d_{2k} - 1/3\delta_{jk}\right)d_{2i} \\
&- Y_G^{11}(h_2)\left(d_{2j}\delta_{ki} + d_{2k}\delta_{ji} - 2d_{2i}d_{2j}d_{2k}\right) \\
&+ X_G^{11}(h_3)\left(d_{3j}d_{3k} - 1/3\delta_{jk}\right)d_{3i} \\
&+ Y_G^{11}(h_3)\left(d_{3j}\delta_{ki} + d_{3k}\delta_{ji} - 2d_{3i}d_{3j}d_{3k}\right) , && (A.29) \\
\tilde{G}_{ijk}^{23} &= -X_G^{12}(h_3)\left(d_{3j}d_{3k} - 1/3\delta_{jk}\right)d_{3i}
\end{aligned}$$

$$- \quad Y_G^{12}(h_3)\left(d_{3j}\delta_{ki} + d_{3k}\delta_{ji} - 2d_{3i}d_{3j}d_{3k}\right) , \tag{A.30}$$

for $i = 1, 2$, $j = 1, 2$, and $k = 3 - j$. The $\tilde{H}$ tensors can be expressed as

$$\tilde{H}^{10}_{ijk} = Y_H^{12}(h_1)\left(\epsilon_{jil}d_{1l}d_{1k} + \epsilon_{kil}d_{1l}d_{1j}\right) , \tag{A.31}$$

$$\tilde{H}^{11}_{ijk} = Y_H^{11}(h_1)\left(\epsilon_{jil}d_{1l}d_{1k} + \epsilon_{kil}d_{1l}d_{1j}\right) + Y_H^{11}(h_2)\left(\epsilon_{jil}d_{2l}d_{2k} + \epsilon_{kil}d_{2l}d_{2j}\right) , \tag{A.32}$$

$$\tilde{H}^{12}_{ijk} = Y_H^{12}(h_2)\left(\epsilon_{jil}d_{2l}d_{2k} + \epsilon_{kil}d_{2l}d_{2j}\right) , \tag{A.33}$$

$$\tilde{H}^{21}_{ijk} = \tilde{H}^{12}_{ijk} , \tag{A.34}$$

$$\tilde{H}^{22}_{ijk} = Y_H^{11}(h_2)\left(\epsilon_{jil}d_{2l}d_{2k} + \epsilon_{kil}d_{2l}d_{2j}\right) + Y_H^{11}(h_3)\left(\epsilon_{jil}d_{3l}d_{3k} + \epsilon_{kil}d_{3l}d_{3j}\right) , \tag{A.35}$$

$$\tilde{H}^{23}_{ijk} = Y_H^{12}(h_3)\left(\epsilon_{jil}d_{3l}d_{3k} + \epsilon_{kil}d_{3l}d_{3j}\right) , \tag{A.36}$$

for $i = 3$, $j = 1, 2$, and $k = 3 - j$.

In the above expressions,

$$\mathbf{d}_1 = \mathbf{r}_1/|\mathbf{r}_1| , \tag{A.37}$$

$$\mathbf{d}_2 = \mathbf{r}_2/|\mathbf{r}_2| , \tag{A.38}$$

$$\mathbf{d}_3 = \mathbf{r}_3/|\mathbf{r}_3| , \tag{A.39}$$

$$\mathbf{r}_1 = (x_1 - x_0, y_1 - y_0, 0) , \tag{A.40}$$

$$\mathbf{r}_2 = (x_2 - x_1, y_2 - y_1, 0) , \tag{A.41}$$

$$\mathbf{r}_3 = (x_3 - x_2, y_3 - y_2, 0) , \tag{A.42}$$

$$h_1 = |\mathbf{r}_1| - 2 , \tag{A.43}$$

$$h_2 = |\mathbf{r}_2| - 2 , \tag{A.44}$$

$$h_3 = |\mathbf{r}_3| - 2 . \tag{A.45}$$

The scalar resistance functions in equations (A.1-A.36) are also taken from Kim & Karrila (1991). When restricted to monosized spheres, and nondimensionsionalized with the scaling described in §3.3, these functions have the form

$$X_A^{11}(h) = \frac{1}{4h} + \frac{9}{40}\ln(\frac{1}{h}) + 0.9954 + \frac{3}{112}h\ln(\frac{1}{h}) , \tag{A.46}$$

$$X_A^{12}(h) = -\frac{1}{4h} - \frac{9}{40}\ln(\frac{1}{h}) - 0.3502 - \frac{3}{112}h\ln(\frac{1}{h}) \; , \tag{A.47}$$

$$Y_A^{11}(h) = \frac{1}{6}\ln(\frac{1}{h}) + 0.9983 \; , \tag{A.48}$$

$$Y_A^{12}(h) = -\frac{1}{6}\ln(\frac{1}{h}) - 0.2737 \; , \tag{A.49}$$

$$Y_B^{11}(h) = \frac{2}{3}\left(-\frac{1}{4}\ln(\frac{1}{h}) + 0.2390 - \frac{1}{8}h\ln(\frac{1}{h})\right) \; , \tag{A.50}$$

$$Y_B^{12}(h) = \frac{2}{3}\left(\frac{1}{4}\ln(\frac{1}{h}) - 0.0017 + \frac{1}{8}h\ln(\frac{1}{h})\right) \; , \tag{A.51}$$

$$Y_C^{11}(h) = \frac{4}{3}\left(\frac{1}{5}\ln(\frac{1}{h}) + 0.7028 + \frac{47}{250}h\ln(\frac{1}{h})\right) \; , \tag{A.52}$$

$$Y_C^{12}(h) = \frac{4}{3}\left(\frac{1}{20}\ln(\frac{1}{h}) - 0.0274 + \frac{31}{500}h\ln(\frac{1}{h})\right) \; , \tag{A.53}$$

$$X_G^{11}(h) = \frac{2}{3}\left(\frac{3}{8h} + \frac{27}{80}\ln(\frac{1}{h}) - 0.469 + \frac{117}{560}h\ln(\frac{1}{h})\right) \; , \tag{A.54}$$

$$X_G^{12}(h) = -\frac{2}{3}\left(\frac{3}{8h} + \frac{27}{80}\ln(\frac{1}{h}) - 0.195 + \frac{117}{560}h\ln(\frac{1}{h})\right) \; , \tag{A.55}$$

$$Y_G^{11}(h) = \frac{2}{3}\left(\frac{1}{8}\ln(\frac{1}{h}) - 0.142 + \frac{1}{16}h\ln(\frac{1}{h})\right) \; , \tag{A.56}$$

$$Y_G^{12}(h) = -\frac{2}{3}\left(\frac{1}{8}\ln(\frac{1}{h}) - 0.103 + \frac{1}{16}h\ln(\frac{1}{h})\right) \; , \tag{A.57}$$

$$Y_H^{11}(h) = \frac{4}{3}\left(\frac{1}{40}\ln(\frac{1}{h}) - 0.074 + \frac{137}{2000}h\ln(\frac{1}{h})\right) \; , \tag{A.58}$$

$$Y_H^{12}(h) = \frac{4}{3}\left(\frac{1}{10}\ln(\frac{1}{h}) - 0.030 + \frac{113}{2000}h\ln(\frac{1}{h})\right) \; . \tag{A.59}$$

Finally, as originally presented in Kim & Karrila (1991), the coefficient in front of the $h\ln(1/h)$ term in the expression for Y_C^{12} is in error. The expression for Y_C^{12} shown above contains the correct coefficient given in Ladd *et al.*(1990).