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纤维悬浮聚合物熔体描述的均一结构多尺度模型*

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通过对纤维悬浮聚合物熔体的可逆和不可逆热力学过程的耦合,建立了分子链弹性哑铃模型与悬浮纤维取向描述相耦合的、具有均一(GENERIC)结构形式的熔体多尺度模型. 由该均一结构的多尺度模型不仅可以得出熔体不同尺度上的应力贡献,还可为一般多尺度模型方程组的建立提供其结构形式均一化的方法.

关键词:GENERIC 结构, 纤维取向, 黏弹性, 聚合物

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1. 引 言

纤维增强高聚物材料的力学行为不仅依赖于成型过程中增强纤维的取向状态和所受外力的情况,还与非平衡态下的温度场有关. GENERIC[1,2](a General Equation for the Non-Equilibrium Reversible-Irreversible Coupling)结构通过把非平衡体系中的大分子链看作处于局部平衡状态的微元体进行系统分析,并将独立状态变量的时间演化过程分成可逆(伴随可逆动力学的 Poisson 算子作用于总能量的泛函导数)和不可逆(伴随耗散过程的 Ginzburg- Landau 算子作用于熵的泛函导数)过程两部分之和.

目前 GENERIC 结构已被应用于复杂流场的非平衡态热力学研究. Ottinger[3]针对一般的动力学方程给出了 GENERIC 结构的映射算子形式,使得 GENERIC 结构具有更宏观的表现形式. Jongschaap 和 Ottinger[4]则给出了驱动热力学系统的 GENERIC 数学表示. 对于开放系统的非平衡态热力学研究,Ottinger[5]也给出了其 GENERIC 结构表式. Grmela[6]还给出了 Euler 场下 Lagrange 流体动力学的 GENERIC 解释. 在聚合物复杂系统模型方面,对蠕动模型[7]和支化聚合物的 Pom-Pom 模型[8,9],GENERIC 结构都有所应用.

在多尺度描述方面,GENERIC 结构并不因所描述系统层次和尺度之间的跳跃而改变. 在该结构中,大尺度信息可以由微小尺度进行推导,因此其具备多尺度描述系统的特性. 由 GENERIC 结构展开可以得到由不同尺度上控制方程所组成的对系统的多尺度描述方程组. 因此,此类型对聚合物熔体的非等温多尺度描述,不仅可以实现多尺度方程组的均一形式表达,还可以得到各尺度上的应力贡献. 故而 GENERIC 结构对非等温聚合物熔体的研究具有非常重要的意义. 为此,本文将基于 GENERIC 结构,构造非等温短纤维悬浮聚合物熔体的均一结构多尺度模型.

2. GENERIC 基本结构

GENERIC[1,2]结构最早是为了描述非平衡态下的复杂流体动力学和热力学过程而建立的一种一般形式. 它提供了一种类似平衡态理论、且可用于表征非平衡态下系统非线性热力学行为的方法. 事实上,复杂流体的流变行为以及松弛现象等都属于非平衡态范畴,但在 GENERIC 之前还没有一种广泛适用于非平衡态的多尺度关联理论.

GENERIC 结构认为任意时间演化方程总可以写为如下形式[2]:

$$\frac{\mathrm{d}x}{\mathrm{d}t} = L\frac{\delta E}{\delta x} + M\frac{\delta S}{\delta x}, \tag{1}$$

其中 x 是描述非平衡系统的独立变量的集合;作为状态变量 x 的函数,$E(x)$和 $S(x)$分别是系统的总

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能量和总熵;L 和 M 可看作是线性算子;$\delta/\delta x$ 是 Volterra 泛函导数.

x 和所选物理场密切相关,其选取一般遵循以下原则:1) 是否可以表征相关的系统特性;2) 是否代表系统恰当的粗粒层次;3) 系统变量是否具有独立性(线性无关性)?

算子 L 和 M 可以分别用 Poisson 括号{}和扩散括号[]表示为[2]

$$\{A,B\}=\left\langle\frac{\delta A}{\delta x},L\frac{\delta B}{\delta x}\right\rangle,\tag{2}$$

$$[A,B]=\left\langle\frac{\delta A}{\delta x},M\frac{\delta B}{\delta x}\right\rangle,\tag{3}$$

其中〈〉表示内积,A 和 B 分别为状态空间中足够正则的实函数. 且算子 L 满足反对称性和 Jacobi 等式[2],即

$$\{A,B\}=-\{B,A\},\tag{4}$$

$$\{A,\{B,C\}\}+\{B,\{C,A\}\}+\{C,\{A,B\}\}=0.\tag{5}$$

算子 M 满足对称性和非负性[2],即

$$[A,B]=[B,A],\tag{6}$$

$$[A,A]\geqslant 0.\tag{7}$$

这样 L 和 M 又称作 Poisson 算子和 Ginzburg-Landau 算子(度量矩阵).

GENERIC 结构还要求具有简并条件[2],即梯度 $\frac{\delta S}{\delta x}$ 和 $\frac{\delta E}{\delta x}$ 分别在 L 和 M 的零空间内,即

$$L\frac{\delta S}{\delta x}=0,\tag{8}$$

$$M\frac{\delta E}{\delta x}=0.\tag{9}$$

前者表示 L 对系统动力学的贡献具有可逆性,后者表示 M 对系统动力学的贡献具有能量守恒性. 因此方程(1)可以看作是由可逆和不可逆两部分贡献之和组成. 这种演化方程的表述方法也叫做双生成元方法.

由(2)和(3)式可以得出任意泛函 A 的时间演化方程可写成如下形式:

$$\frac{\mathrm{d}A}{\mathrm{d}t}=\{A,E\}+[A,S].\tag{10}$$

利用简并条件(9)以及 L 和 M 的反对称性(4)和对称性(6),可以得出能量的守恒关系

$$\frac{\mathrm{d}E}{\mathrm{d}t}=\{E,E\}+[E,S]=0.\tag{11}$$

再利用 M 的非负性(7),可以得出熵增关系

$$\frac{\mathrm{d}S}{\mathrm{d}t}=\{S,E\}+[S,S]\geqslant 0.\tag{12}$$

因此 GENERIC 结构包含了热力学第一、第二定律,加上 L 和 M 所满足的时间-结构不变性(5)和 Onsager 关系(6),可知 GENERIC 结构满足热力学一致性原则和热力学基本原理.

推导系统的 GENERIC 结构,需要以下几个步骤:

1) 选取恰当的状态变量 x;

2) 确定系统的总能量 E 和熵 S;

3) 根据 x 的变换行为、能量耗散形式,L 和 M 的性质以及简并条件,确定算子 L 和 M 的具体表达式.

3. 聚合物熔体描述的均一结构多尺度模型

对于无纤维悬浮的聚合物溶液,使用描述聚合物大分子链的粗粒弹性哑铃模型对聚合物微观分子链信息进行描述,则系统状态变量可选取为 $x=\{\rho,\boldsymbol{u},\varepsilon,\phi\}$,这里 $\rho(\boldsymbol{r})$ 为质量密度、$\boldsymbol{u}(\boldsymbol{r})$ 为动量密度、$\varepsilon(\boldsymbol{r})$ 为内能密度,$\phi(\boldsymbol{r},\boldsymbol{Q})$ 为分子链哑铃模型的概率分布函数. 其中 $\boldsymbol{u}(\boldsymbol{r})$ 和速度场 $\boldsymbol{v}(\boldsymbol{r})$ 相关,即 $\boldsymbol{u}(\boldsymbol{r})=\rho(\boldsymbol{r})\boldsymbol{v}(\boldsymbol{r})$,$\boldsymbol{r}$ 和 $\boldsymbol{Q}$ 分别表示空间位置向量和哑铃构型向量.

无纤维悬浮聚合物溶液系统的总能量和熵可以写为[2]

$$E=\int\left[\frac{1}{2}\frac{\boldsymbol{u}(\boldsymbol{r})^2}{\rho(\boldsymbol{r})}+\varepsilon(\boldsymbol{r})+\int V(Q)\phi(\boldsymbol{r},\boldsymbol{Q})\mathrm{d}^3Q\right]\mathrm{d}^3r,\tag{13}$$

$$S=\int\left\{s(\rho(\boldsymbol{r}),\varepsilon(\boldsymbol{r}))-\int\phi(\boldsymbol{r},\boldsymbol{Q})\left[\frac{V^{\mathrm{S}}(\boldsymbol{r},Q)}{T(\boldsymbol{r})}+k\ln\phi(\boldsymbol{r},\boldsymbol{Q})\right]\mathrm{d}^3Q\right\}\mathrm{d}^3r,\tag{14}$$

其中 $V(Q)$ 是哑铃两链珠间的相互作用势,即弹簧势,$V^{\mathrm{S}}(\boldsymbol{r},Q)$ 是依赖于局部温度的熵源弹簧势,$s(\rho(\boldsymbol{r}),\varepsilon(\boldsymbol{r}))$ 是牛顿溶剂的熵,k 为 Boltzman 常数,$\phi\ln\phi$ 与哑铃平移熵和构型熵相关.

通过总能量 E 和熵 S 的表达式(13),(14),可以写出

$$\frac{\delta E}{\delta x}=\begin{pmatrix}\dfrac{\delta}{\delta\rho(\boldsymbol{r})}\\[2mm]\dfrac{\delta}{\delta\boldsymbol{u}(\boldsymbol{r})}\\[2mm]\dfrac{\delta}{\delta\varepsilon(\boldsymbol{r})}\\[2mm]\dfrac{\delta}{\delta\phi(\boldsymbol{r},\boldsymbol{Q})}\end{pmatrix}E(\rho,\boldsymbol{u},\varepsilon,\phi)$$

$$= \begin{pmatrix} -\frac{1}{2}\boldsymbol{v}(\boldsymbol{r})^2 \\ \boldsymbol{v}(\boldsymbol{r}) \\ 1 \\ V(\boldsymbol{Q}) \end{pmatrix}, \tag{15}$$

$$\frac{\delta S}{\delta x} = \begin{pmatrix} \dfrac{\delta}{\delta\rho(\boldsymbol{r})} \\ \dfrac{\delta}{\delta\boldsymbol{u}(\boldsymbol{r})} \\ \dfrac{\delta}{\delta\varepsilon(\boldsymbol{r})} \\ \dfrac{\delta}{\delta\phi(\boldsymbol{r},\boldsymbol{Q})} \end{pmatrix} S(\rho,\boldsymbol{u},\varepsilon,\phi)$$

$$= \begin{pmatrix} -\dfrac{\mu(\boldsymbol{r})}{T(\boldsymbol{r})} \\ 0 \\ \dfrac{1}{T(\boldsymbol{r})} \\ -\dfrac{V^{S}(\boldsymbol{r},\boldsymbol{Q})}{T(\boldsymbol{r})} - k\ln\phi(\boldsymbol{r},\boldsymbol{Q}) - k \end{pmatrix}, \tag{16}$$

其中温度 T 和局部化学势 μ 分别定义为

$$T(\boldsymbol{r}) = \left(\frac{\partial s(\rho,\varepsilon)}{\partial\varepsilon}\right)^{-1},$$

$$\frac{\mu(\boldsymbol{r})}{T(\boldsymbol{r})} = -\frac{\partial s(\rho,\varepsilon)}{\partial\rho}.$$

3.1. 构建 Poisson 算子 L

$x = \{\rho,\boldsymbol{u},\varepsilon,\phi\}$ 中质量密度 $\rho(\boldsymbol{r})$ 的变换行为[2]

$$\rho(\boldsymbol{r}) \to \rho(\boldsymbol{r}) - t\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\rho(\boldsymbol{r})], \tag{17}$$

来源于标量密度场 $\rho(\boldsymbol{r}) \to \rho(\boldsymbol{r} - t\boldsymbol{v}(\boldsymbol{r}))\left|\boldsymbol{I} - t\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right|$ 关于 t 的一阶截断项($\boldsymbol{I}$ 表示单位向量). 类似地,协变向量密度场 $\boldsymbol{u}(\boldsymbol{r})$ 的变换行为[2]

$$\boldsymbol{u}(\boldsymbol{r}) \to \boldsymbol{u}(\boldsymbol{r}) - t\left\{\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{r})] + \left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\cdot\boldsymbol{u}(\boldsymbol{r})\right\}. \tag{18}$$

内能密度场 $\varepsilon(\boldsymbol{r})$ 的变化行为[2]为

$$\varepsilon(\boldsymbol{r}) \to \varepsilon(\boldsymbol{r}) - t\left\{\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\varepsilon(\boldsymbol{r})] + [p(\boldsymbol{r})\boldsymbol{I} + \boldsymbol{\Pi}(\boldsymbol{r})] : \frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right\}. \tag{19}$$

不考虑弹簧熵的守恒性,其中哑铃链珠带来的渗透压力[2]为

$$\boldsymbol{\Pi}(\boldsymbol{r}) = \int\phi(\boldsymbol{r},\boldsymbol{Q})\left[2kT(\boldsymbol{r})\boldsymbol{I} - \boldsymbol{Q}\frac{\partial V^{S}(\boldsymbol{r},\boldsymbol{Q})}{\partial\boldsymbol{Q}}\right]\mathrm{d}^3 Q. \tag{20}$$

基于 ϕ 在 r 上是标量密度,且 $\boldsymbol{Q}$ 作为逆变向量,构型分布函数 $\phi(\boldsymbol{r},\boldsymbol{Q})$ 的变换行为[2]为

$$\phi(\boldsymbol{r},\boldsymbol{Q}) \to \phi(\boldsymbol{r},\boldsymbol{Q}) - t\left\{\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\phi(\boldsymbol{r},\boldsymbol{Q})] + \frac{\partial}{\partial\boldsymbol{Q}}\cdot\left[\left(\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right)^{\mathrm{T}}\cdot\boldsymbol{Q}\phi(\boldsymbol{r},\boldsymbol{Q})\right]\right\}. \tag{21}$$

对于流体动力学的一般形式,Poisson 算子 L 有两个离散指标(对应于独立状态变量集合里分量的数目 q)和两个标号(对应于空间位置),因此可以记作 $L(\boldsymbol{r},\boldsymbol{r}')$. L 的乘积不仅包含 $q\times q$ 矩阵的乘积,还包含 r' 上的积分. 当考虑聚合物分子链构象时,L 成为了更大级数的矩阵 $L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{r}',\boldsymbol{Q}')$,且 L 的乘积包含 Q' 上的积分.

因为(8),(4)式和 $L\frac{\delta E}{\delta x}$ 仅反映系统可逆过程,由

$$\begin{pmatrix} -\dfrac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\rho(\boldsymbol{r})] \\ -\dfrac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{r})] - \left[\dfrac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\cdot\boldsymbol{u}(\boldsymbol{r}) \\ -\dfrac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\varepsilon(\boldsymbol{r})] - [p(\boldsymbol{r})\boldsymbol{I} + \boldsymbol{\Pi}(\boldsymbol{r})] : \dfrac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r}) \\ -\dfrac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\phi(\boldsymbol{r},\boldsymbol{Q})] - \dfrac{\partial}{\partial\boldsymbol{Q}}\cdot\left[\left(\dfrac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right)^{\mathrm{T}}\cdot\boldsymbol{Q}\phi(\boldsymbol{r},\boldsymbol{Q})\right] \end{pmatrix} = \int L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{r}',\boldsymbol{Q}')\cdot\begin{pmatrix} \dfrac{\delta G}{\delta\rho(\boldsymbol{r}')} \\ \dfrac{\delta G}{\delta\boldsymbol{u}(\boldsymbol{r}')} \\ \dfrac{\delta G}{\delta\varepsilon(\boldsymbol{r}')} \\ \displaystyle\int\frac{\delta G}{\delta\phi(\boldsymbol{r}',\boldsymbol{Q}')}\mathrm{d}^3 Q' \end{pmatrix}\mathrm{d}^3 r',$$

其中 $G = \int\boldsymbol{u}(\boldsymbol{r})\cdot\boldsymbol{v}(\boldsymbol{r}))\mathrm{d}^3 r$ 是协变向量 $\boldsymbol{u}(\boldsymbol{r})$ 和逆变向量 $\boldsymbol{v}(\boldsymbol{r})$ 的双线性函数,可得

$$
L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{r}',\boldsymbol{Q}')=\begin{pmatrix}
0 & \rho(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'} & 0 & 0\\
\rho(\boldsymbol{r})\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'} & \begin{array}{l}\boldsymbol{u}(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{u}(\boldsymbol{r})\end{array} & \begin{array}{l}\varepsilon(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ \cdot[p(\boldsymbol{r}')\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r}')]\end{array} & \begin{array}{l}\phi(\boldsymbol{r},\boldsymbol{Q}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ -\dfrac{\partial}{\partial\boldsymbol{Q}'}\Big[\phi(\boldsymbol{r}',\boldsymbol{Q}')\boldsymbol{Q}'\\ \cdot\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\Big]\end{array}\\
0 & \begin{array}{l}\varepsilon(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ \cdot[p(\boldsymbol{r}')\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r}')]\end{array} & 0 & 0\\
0 & \begin{array}{l}\phi(\boldsymbol{r}',\boldsymbol{Q})\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\dfrac{\partial}{\partial\boldsymbol{Q}}\Big[\phi(\boldsymbol{r},\boldsymbol{Q})\boldsymbol{Q}\\ \cdot\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial(\boldsymbol{r}')}\Big]\end{array} & 0 & 0
\end{pmatrix}.
$$

经 r' 上的积分后,得

$$
L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{Q}')=\begin{pmatrix}
0 & \dfrac{\partial}{\partial\boldsymbol{r}}\rho(\boldsymbol{r}) & 0 & 0\\
\rho(\boldsymbol{r})\dfrac{\partial}{\partial\boldsymbol{r}} & \left[\dfrac{\partial}{\partial\boldsymbol{r}}\boldsymbol{u}(\boldsymbol{r})+\boldsymbol{u}(\boldsymbol{r})\dfrac{\partial}{\partial\boldsymbol{r}}\right]^{\mathrm{T}} & \begin{array}{l}\varepsilon(\boldsymbol{r})\dfrac{\partial}{\partial\boldsymbol{r}}+\dfrac{\partial}{\partial\boldsymbol{r}}p(\boldsymbol{r})\\ +\dfrac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{\Pi}(\boldsymbol{r})\end{array} & \begin{array}{l}\phi(\boldsymbol{r},\boldsymbol{Q}')\dfrac{\partial}{\partial\boldsymbol{r}}\\ -\dfrac{\partial}{\partial\boldsymbol{r}}\cdot\phi(\boldsymbol{r},\boldsymbol{Q}')\boldsymbol{Q}'\dfrac{\partial}{\partial\boldsymbol{Q}'}\end{array}\\
0 & \begin{array}{l}\dfrac{\partial}{\partial\boldsymbol{r}}\varepsilon(\boldsymbol{r})\\ +p(\boldsymbol{r})\dfrac{\partial}{\partial\boldsymbol{r}}+\boldsymbol{\Pi}(\boldsymbol{r})\cdot\dfrac{\partial}{\partial\boldsymbol{r}}\end{array} & 0 & 0\\
0 & \begin{array}{l}\dfrac{\partial}{\partial\boldsymbol{r}}\phi(\boldsymbol{r},\boldsymbol{Q})\\ +\dfrac{\partial}{\partial\boldsymbol{Q}}\phi(\boldsymbol{r},\boldsymbol{Q})\boldsymbol{Q}\cdot\dfrac{\partial}{\partial\boldsymbol{r}}\end{array} & 0 & 0
\end{pmatrix}.
\tag{22}
$$

3.2. 构建度量矩阵 M

由于 M 是不可逆过程的算子,因此 M 第一列元素为零(质量守恒方程中只有可逆过程). 根据对称性,第一行元素也全部为零.

首先通过哑铃构型空间的一般扩散行为确定右下角元素,其他非零元素通过(9)式和对称性(6)式得到.

在哑铃构型空间的一般扩散行为

$$
\frac{\partial}{\partial\boldsymbol{Q}}\left[\frac{2}{\zeta}\left(\frac{\partial V}{\partial\boldsymbol{Q}}+\frac{\partial V^{\mathrm{S}}}{\partial\boldsymbol{Q}}\right)\phi\right]
+\frac{\partial}{\partial\boldsymbol{r}}\cdot\frac{kT}{2\zeta}\frac{\partial\phi}{\partial\boldsymbol{r}}+\frac{\partial}{\partial\boldsymbol{Q}}\cdot\frac{2kT}{\zeta}\frac{\partial\phi}{\partial\boldsymbol{Q}}
\tag{23}
$$

中,第一项为弹簧弹力引起的贡献(这里在弹力 F 的定义中考虑了弹簧对熵的贡献),第二项是非平衡态下的熵引起的贡献,最后一项为 Brown 力带来的贡献.

考虑到$\dfrac{\delta S}{\delta x}$的分量,可以先得到 M 的右下角元素为

$$
-\frac{\partial}{\partial\boldsymbol{Q}}\cdot\frac{2T}{\zeta}\phi(\boldsymbol{r},\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{Q}-\boldsymbol{Q}')}{\partial\boldsymbol{Q}}
-\frac{\partial}{\partial\boldsymbol{r}}\cdot\frac{T}{2\zeta}\phi(\boldsymbol{r},\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{Q}-\boldsymbol{Q}')}{\partial\boldsymbol{r}}.
\tag{24}
$$

根据简并条件以及对称性,最后得到

$$
M(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{Q}')=\begin{pmatrix}
0 & 0 & 0 & 0\\
0 & \begin{array}{l}-\left(\frac{\partial}{\partial \boldsymbol{r}}\eta_{\mathrm{s}}T\frac{\partial}{\partial \boldsymbol{r}}\right)^{\mathrm{T}}\\ -\boldsymbol{I}\frac{\partial}{\partial \boldsymbol{r}}\cdot\eta_{\mathrm{s}}T\frac{\partial}{\partial \boldsymbol{r}}\end{array} & \frac{\partial}{\partial \boldsymbol{r}}\cdot\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}} & 0\\
0 & -\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}}\frac{\partial}{\partial \boldsymbol{r}} & \begin{array}{l}\frac{1}{2}\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}}-\frac{\partial}{\partial \boldsymbol{r}}\cdot k_{\mathrm{p}}T^{2}\frac{\partial}{\partial \boldsymbol{r}}\\ +\frac{2T}{\zeta}\int\left(\frac{\partial V}{\partial \boldsymbol{Q}}\right)^{2}\phi(\boldsymbol{r},\boldsymbol{Q})\mathrm{d}^{3}Q\end{array} & -\frac{2T}{\zeta}\frac{\partial V}{\partial \boldsymbol{Q}}\cdot\phi(\boldsymbol{r},\boldsymbol{Q}')\frac{\partial}{\partial \boldsymbol{Q}'}\\
0 & 0 & \frac{\partial}{\partial \boldsymbol{Q}}\cdot\frac{2T}{\zeta}\frac{\partial V}{\partial \boldsymbol{Q}}\cdot\phi(\boldsymbol{r},\boldsymbol{Q}) & \begin{array}{l}-\frac{\partial}{\partial \boldsymbol{Q}}\cdot\frac{2T}{\zeta}\phi(\boldsymbol{r},\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{Q}-\boldsymbol{Q}')}{\partial \boldsymbol{Q}}\\ -\frac{\partial}{\partial \boldsymbol{r}}\cdot\frac{T}{2\zeta}\phi(\boldsymbol{r},\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{Q}-\boldsymbol{Q}')}{\partial \boldsymbol{r}}\end{array}
\end{pmatrix},\tag{25}
$$

其中，k_p，ζ 分别为热导率和哑铃摩擦系数.

事实上，度量矩阵 M 多数凭经验获得. 由于任何形式非平衡态下的演化方程都可写成 GENERIC 的形式，所以根据已有成熟的独立变量的方程组，如经典流体力学时间演化方程[2]，可以得出对应的算子 L 和 M. 加入其他独立变量后的 GENERIC 形式，尤其是度量矩阵 M，可以在经典力学对应算子 M 的基础上进行拓展得到.

这样经由 GENERIC 结构，通过状态变量 $x=\{\rho,\boldsymbol{u},\varepsilon,\phi\}$，总能量 E 和熵 S 的泛函形式(15)，(16)，以及算子 L(22)式和 M(25)式，可以展开得到非平衡态下的基于大分子哑铃概率分布函数描述的聚合物多尺度方程组[2]

$$
\frac{\partial\rho}{\partial t}=-\frac{\partial}{\partial \boldsymbol{r}}(\boldsymbol{v}\rho),\tag{26}
$$

$$
\frac{\partial \boldsymbol{u}}{\partial t}=-\frac{\partial}{\partial \boldsymbol{r}}\cdot(\boldsymbol{v}\boldsymbol{u})-\frac{\partial}{\partial \boldsymbol{r}}\left(p+2kT\int\phi\mathrm{d}^{3}Q\right)+\frac{\partial}{\partial \boldsymbol{r}}\cdot\eta_{\mathrm{s}}\dot{\boldsymbol{\gamma}}+\frac{\partial}{\partial \boldsymbol{r}}\cdot\int\boldsymbol{Q}\left(\frac{\partial V}{\partial \boldsymbol{Q}}+\frac{\partial V^{\mathrm{S}}}{\partial \boldsymbol{Q}}\right)\phi\mathrm{d}^{3}Q,\tag{27}
$$

$$
\begin{aligned}
\frac{\partial\varepsilon}{\partial t}=&-\frac{\partial}{\partial \boldsymbol{r}}\cdot(\boldsymbol{v}\varepsilon)+\frac{\partial}{\partial \boldsymbol{r}}\cdot k_{\mathrm{p}}\frac{\partial T}{\partial \boldsymbol{r}}\\
&+\frac{1}{2}\eta_{\mathrm{s}}\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}}-\frac{1}{2}(p\boldsymbol{I}+\boldsymbol{\Pi}):\dot{\boldsymbol{\gamma}}\\
&+\frac{2}{\zeta}\int\frac{\partial V}{\partial \boldsymbol{Q}}\cdot\left(\frac{\partial V}{\partial \boldsymbol{Q}}+\frac{\partial V^{\mathrm{S}}}{\partial \boldsymbol{Q}}\right)\phi\mathrm{d}^{3}Q\\
&-\frac{2kT}{\zeta}\int\phi\frac{\partial}{\partial \boldsymbol{Q}}\cdot\frac{\partial V}{\partial \boldsymbol{Q}}\mathrm{d}^{3}Q,
\end{aligned}\tag{28}
$$

$$
\begin{aligned}
\frac{\partial\psi}{\partial t}=&-\frac{\partial}{\partial \boldsymbol{r}}\cdot(\boldsymbol{v}\phi)-\frac{\partial}{\partial \boldsymbol{Q}}\left[\left[\frac{\partial \boldsymbol{v}^{\mathrm{T}}}{\partial \boldsymbol{r}}\cdot\boldsymbol{Q}\right.\right.\\
&\left.\left.-\frac{2}{\zeta}\left(\frac{\partial V}{\partial \boldsymbol{Q}}+\frac{\partial V^{\mathrm{S}}}{\partial \boldsymbol{Q}}\right)\right]\phi\right\}\\
&+\frac{\partial}{\partial \boldsymbol{r}}\cdot\frac{kT}{2\zeta}\frac{\partial\phi}{\partial \boldsymbol{r}}+\frac{\partial}{\partial \boldsymbol{Q}}\cdot\frac{2kT}{\zeta}\frac{\partial\phi}{\partial \boldsymbol{Q}}.
\end{aligned}\tag{29}
$$

可以看出，(26)式即经典流体力学的连续方程，对不可压缩假设，即$\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{r}}=0$；(27)式即动量方程，其中

$$
\boldsymbol{\tau}_{\mathrm{p}}=-2kT\int\phi\mathrm{d}^{3}Q+\int\boldsymbol{Q}\left(\frac{\partial V}{\partial \boldsymbol{Q}}+\frac{\partial V^{\mathrm{S}}}{\partial \boldsymbol{Q}}\right)\phi\mathrm{d}^{3}Q.\tag{30}
$$

(28)式是内能密度的演化方程，其中不仅包含了应力的贡献，还包含了能量耗散的形式；(29)式是哑铃概率分布函数的演化方程，除增加了非平衡态项

$$
\frac{\partial}{\partial \boldsymbol{r}}\cdot\frac{kT}{2\zeta}\frac{\partial\phi}{\partial \boldsymbol{r}}\tag{31}
$$

外，与平衡态下的演化方程相同.

4. 纤维悬浮聚合物熔体描述的均一结构多尺度模型

考虑到纤维取向对材料性能的重要作用，这里选用纤维取向张量描述的纤维取向概率分布函数分析圆柱纤维取向对材料性能的影响. 纤维取向张量 $\boldsymbol{a}_2$，$\boldsymbol{a}_4$，… 的分量 a_{ij}，a_{ijkl}，… 定义为 $a_{ij\cdots}=\int_{S^2}p_ip_j\cdots\psi(\theta,\phi)\mathrm{d}S$，其中 $\boldsymbol{p}$ 是单根纤维的单位向量，作为加权函数使用的 $\psi(\theta,\phi)$ 是纤维构象分布函数.

4.1. 基于概率分布函数的均一结构多尺度模型

对聚合物分子链进行近似的哑铃模型中，概率分布函数 $\phi(r,Q)$ 反映了哑铃模型的构象以及分布情况，对于表述分子链构象空间与物理空间之间的

关系非常重要. 因此这里仍选用哑铃模型的概率分布函数 $\phi(\boldsymbol{r},\boldsymbol{Q})$ 对聚合物分子链进行描述,则纤维悬浮聚合物熔体的独立变量可选取为 $x=\{\rho,\boldsymbol{u},\varepsilon,\phi,\boldsymbol{a}_2\}$. 记 $e_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)$ 和 $s_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)$ 分别为纤维取向引起的能量贡献和熵贡献,则总能量 E 和熵 S 可表示为

$$E=\int\Big[\frac{1}{2}\frac{\boldsymbol{u}(\boldsymbol{r})^2}{\rho(\boldsymbol{r})}+\varepsilon(\boldsymbol{r})+\int V(Q)\phi(\boldsymbol{r},\boldsymbol{Q})\mathrm{d}^3Q+e_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)\Big]\mathrm{d}^3r,\tag{32}$$

$$S=\int\Big\{s(\rho(\boldsymbol{r}),\varepsilon(\boldsymbol{r}))-\int\phi(\boldsymbol{r},\boldsymbol{Q})\Big[\frac{V(\boldsymbol{r},Q)}{T(\boldsymbol{r})}+k\ln\phi(\boldsymbol{r},\boldsymbol{Q})\Big]\mathrm{d}^3Q+s_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)\Big\}\mathrm{d}^3r.\tag{33}$$

这样,

$$\frac{\delta E}{\delta x}=\begin{pmatrix}-\frac{1}{2}\boldsymbol{v}(\boldsymbol{r})^2\\ \boldsymbol{v}(\boldsymbol{r})\\ 1\\ V(Q)\\ \frac{\partial e_{\mathrm{f}}}{\partial\boldsymbol{a}_2(\boldsymbol{r})}\end{pmatrix},\tag{34}$$

$$\frac{\delta S}{\delta x}=\begin{pmatrix}-\frac{\mu(\boldsymbol{r})}{T(\boldsymbol{r})}\\ 0\\ \frac{1}{T(\boldsymbol{r})}\\ -\frac{V(\boldsymbol{r},\boldsymbol{Q})}{T(\boldsymbol{r})}-k\ln\phi(\boldsymbol{r},\boldsymbol{Q})-k\\ \frac{\partial s_{\mathrm{f}}}{\partial\boldsymbol{a}_2(\boldsymbol{r})}\end{pmatrix},\tag{35}$$

取向张量 $a_2(r)$ 作为反映短纤维取向的逆变张量,其变化形式为

$$\begin{aligned}\boldsymbol{a}_2(\boldsymbol{r})\to\boldsymbol{a}_2(\boldsymbol{r})-t\Big\{&\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{a}_2(\boldsymbol{r})]\\&-\frac{1}{2}(\chi-1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]^{\mathrm{T}}\cdot\boldsymbol{a}_2\\&-\frac{1}{2}(\chi+1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]\cdot\boldsymbol{a}_2\\&-\frac{1}{2}\boldsymbol{a}_2\cdot(\chi+1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]^{\mathrm{T}}\\&-\frac{1}{2}\boldsymbol{a}_2\cdot(\chi-1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]\Big\},\end{aligned}\tag{36}$$

其中 $\chi=(\lambda^2-1)/(\lambda^2+1)$ 是关于纤维长径比 $\lambda=L/D$ 的参数. 经由

$$\begin{pmatrix}-\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\rho(\boldsymbol{r})]\\ -\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{r})]-\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]\cdot\boldsymbol{u}(\boldsymbol{r})\\ -\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\varepsilon(\boldsymbol{r})]-[p(\boldsymbol{r})\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r})]:\frac{\partial}{\partial\boldsymbol{v}}\boldsymbol{v}(\boldsymbol{r})\\ -\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\phi(\boldsymbol{r},\boldsymbol{Q})]-\frac{\partial}{\partial\boldsymbol{Q}}\cdot\Big[\Big(\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big)^{\mathrm{T}}\cdot\boldsymbol{Q}\phi(\boldsymbol{r},\boldsymbol{Q})\Big]\\ \Big\{-\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{a}_2(\boldsymbol{r})]+\frac{1}{2}(\chi-1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]^{\mathrm{T}}\cdot\boldsymbol{a}_2+\frac{1}{2}(\chi+1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]\cdot\boldsymbol{a}_2\\ +\frac{1}{2}\boldsymbol{a}_2\cdot(\chi+1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]^{\mathrm{T}}+\frac{1}{2}\boldsymbol{a}_2\cdot(\chi-1)\Big[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\Big]\Big\}\end{pmatrix}$$

$$=\int L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{r}',\boldsymbol{Q}')\cdot\begin{pmatrix}\frac{\delta G}{\delta\rho(\boldsymbol{r}')}\\ \frac{\delta G}{\delta\boldsymbol{u}(\boldsymbol{r}')}\\ \frac{\delta G}{\delta\varepsilon(\boldsymbol{r}')}\\ \int\frac{\delta G}{\delta\phi(\boldsymbol{r}',\boldsymbol{Q}')}\mathrm{d}^3Q'\\ \frac{\delta G}{\delta\boldsymbol{a}_2(\boldsymbol{r}')}\end{pmatrix}\mathrm{d}^3\boldsymbol{r}',$$

可得

$$L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{r}',\boldsymbol{Q}')=\begin{pmatrix} 0 & \rho(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'} & 0 & 0 & 0 \\ \rho(\boldsymbol{r})\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'} & \begin{matrix}\boldsymbol{u}(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\+\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{u}(\boldsymbol{r})\end{matrix} & \begin{matrix}\varepsilon(\boldsymbol{r})\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\+\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\\cdot[p(\boldsymbol{r}')\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r}')]\end{matrix} & L_{24} & L_{25} \\ 0 & \begin{matrix}\varepsilon(\boldsymbol{r}')\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\+\dfrac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\\cdot[p(\boldsymbol{r}')\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r}')]\end{matrix} & 0 & 0 & 0 \\ 0 & L_{42} & 0 & 0 & 0 \\ 0 & L_{52} & 0 & 0 & 0 \end{pmatrix},$$

$$L_{24}=\phi(\boldsymbol{r},\boldsymbol{Q}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{\partial}{\partial\boldsymbol{Q}}\left[\phi(\boldsymbol{r}',\boldsymbol{Q}')\boldsymbol{Q}'\cdot\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\right],$$

$$L_{25}=\boldsymbol{a}_2(\boldsymbol{r})\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{a}_2(\boldsymbol{r}')$$
$$-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}')-\frac{1}{2}(\chi-1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}'),$$

$$L_{42}=\phi(\boldsymbol{r}',\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}+\frac{\partial}{\partial\boldsymbol{Q}}\left[\phi(\boldsymbol{r},\boldsymbol{Q})\boldsymbol{Q}\cdot\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\right],$$

$$L_{52}=\boldsymbol{a}_2(\boldsymbol{r}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r}')\cdot\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{a}_2(\boldsymbol{r})$$
$$-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}')-\frac{1}{2}(\chi-1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}').$$

经 r' 上的积分后，

$$L(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{Q}')=\begin{pmatrix} 0 & \dfrac{\partial\delta}{\partial\boldsymbol{r}}\rho(\boldsymbol{r}) & 0 & 0 & 0 \\ \rho(\boldsymbol{r})\dfrac{\partial\delta}{\partial\boldsymbol{r}} & \left(\dfrac{\partial\delta}{\partial\boldsymbol{r}}\boldsymbol{u}(\boldsymbol{r})+\boldsymbol{u}(\boldsymbol{r})\dfrac{\partial\delta}{\partial\boldsymbol{r}}\right]^{\mathrm{T}} & \begin{matrix}\varepsilon(\boldsymbol{r})\dfrac{\partial}{\partial\boldsymbol{r}}\\+\dfrac{\partial}{\partial\boldsymbol{r}}p(\boldsymbol{r})+\dfrac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{\Pi}(\boldsymbol{r})\end{matrix} & L_{24} & L_{25} \\ 0 & \begin{matrix}\dfrac{\partial}{\partial\boldsymbol{r}}\varepsilon(\boldsymbol{r})+p(\boldsymbol{r})\dfrac{\partial}{\partial\boldsymbol{r}}\\+\boldsymbol{\Pi}(\boldsymbol{r})\cdot\dfrac{\partial}{\partial\boldsymbol{r}}\end{matrix} & 0 & 0 & 0 \\ 0 & L_{42} & 0 & 0 & 0 \\ 0 & L_{52} & 0 & 0 & 0 \end{pmatrix},\tag{37}$$

$$L_{24}=\phi(\boldsymbol{r},\boldsymbol{Q}')\frac{\partial}{\partial\boldsymbol{r}}-\frac{\partial}{\partial\boldsymbol{r}}\cdot\phi(\boldsymbol{r},\boldsymbol{Q}')\boldsymbol{Q}'\frac{\partial}{\partial\boldsymbol{Q}'},$$

$$L_{25}=\boldsymbol{a}_2(\boldsymbol{r})\frac{\partial}{\partial\boldsymbol{r}}-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}}-\frac{1}{2}(\chi+1)\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{a}_2(\boldsymbol{r})$$
$$-\frac{1}{2}(\chi+1)\frac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{a}_2(\boldsymbol{r})-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}},$$

$$L_{42}=\frac{\partial}{\partial\boldsymbol{r}}\phi(\boldsymbol{r},\boldsymbol{Q})+\frac{\partial}{\partial\boldsymbol{Q}}\phi(\boldsymbol{r},\boldsymbol{Q})\boldsymbol{Q}\cdot\frac{\partial}{\partial\boldsymbol{r}},$$

$$L_{52}=\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{a}_2(\boldsymbol{r})-\frac{1}{2}(\chi-1)\frac{\partial}{\partial \boldsymbol{r}}\cdot\boldsymbol{a}_2(\boldsymbol{r})-\frac{1}{2}(\chi+1)\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{a}_2(\boldsymbol{r})$$
$$-\frac{1}{2}(\chi+1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial}{\partial \boldsymbol{r}}-\frac{1}{2}(\chi-1)\frac{\partial}{\partial \boldsymbol{r}}\cdot\boldsymbol{a}_2(\boldsymbol{r}).$$

在纤维悬浮聚合物溶液中,渗透压力张量 $\boldsymbol{\Pi}$ 选用满足简并条件(8)的表达式:

$$\boldsymbol{\Pi}(\boldsymbol{r})=\int\phi(\boldsymbol{r},\boldsymbol{Q})\left[2kT(\boldsymbol{r})\boldsymbol{I}-\boldsymbol{Q}\frac{\partial V^{\mathrm{S}}(\boldsymbol{r},\boldsymbol{Q})}{\partial \boldsymbol{Q}}\right]\mathrm{d}^3Q$$
$$+\boldsymbol{\Pi}'(\boldsymbol{r}),$$

其中 $\boldsymbol{\Pi}'(\boldsymbol{r})$ 满足

$$\frac{1}{T}\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{\Pi}'(\boldsymbol{r})+L_{25}\frac{\partial s_{\mathrm{f}}}{\partial \boldsymbol{a}_2(\boldsymbol{r})}=0. \tag{38}$$

根据描述纤维取向的扩散行为表达式 $2D_{\mathrm{r}}(\boldsymbol{I}-m\cdot\boldsymbol{a}_2)$(其中 D_{r} 和 m 分别为反映纤维旋转扩散率的系数和纤维取向空间的维数)以及 $s_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)$ 的表达式,可确定度量矩阵 M 的右下角元素,M 最后一行上其他非零元素通过简并条件和 $e_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)$ 的表达式获得,即

$$M(\boldsymbol{r},\boldsymbol{Q},\boldsymbol{Q}')=\begin{pmatrix}0 & 0 & 0 & 0 & 0\\ 0 & -\left(\frac{\partial}{\partial \boldsymbol{r}}\eta_{\mathrm{s}}T\frac{\partial}{\partial \boldsymbol{r}}\right)^{\mathrm{T}}-\boldsymbol{I}\frac{\partial}{\partial \boldsymbol{r}}\cdot\eta_{\mathrm{s}}T\frac{\partial}{\partial \boldsymbol{r}} & \frac{\partial}{\partial \boldsymbol{r}}\cdot\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}} & 0 & M_{25}\\ 0 & -\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}}\cdot\frac{\partial}{\partial \boldsymbol{r}} & M_{33} & M_{34} & 0\\ 0 & 0 & M_{43} & M_{44} & 0\\ 0 & M_{52} & 0 & 0 & M_{55}\end{pmatrix}, \tag{39}$$

$$M_{33}=\frac{1}{2}\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}}-\frac{\partial}{\partial \boldsymbol{r}}\cdot k_{\mathrm{p}}T^2\frac{\partial}{\partial \boldsymbol{r}}$$
$$+\frac{2T}{\zeta}\int\left(\frac{\partial V}{\partial \boldsymbol{Q}}\right)^2\phi(\boldsymbol{r},\boldsymbol{Q})\mathrm{d}^3Q,$$
$$M_{34}=-\frac{2T}{\zeta}\frac{\partial V}{\partial \boldsymbol{Q}}\cdot\phi(\boldsymbol{r},\boldsymbol{Q}')\frac{\partial}{\partial \boldsymbol{Q}'},$$
$$M_{43}=\frac{\partial}{\partial \boldsymbol{Q}}\cdot\frac{2T}{\zeta}\frac{\partial V}{\partial \boldsymbol{Q}}\cdot\phi(\boldsymbol{r},\boldsymbol{Q}),$$
$$M_{44}=-\frac{\partial}{\partial \boldsymbol{Q}}\cdot\frac{2T}{\zeta}\phi(\boldsymbol{r},\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{Q}-\boldsymbol{Q}')}{\partial \boldsymbol{Q}}$$
$$-\frac{\partial}{\partial \boldsymbol{r}}\cdot\frac{T}{2\zeta}\phi(\boldsymbol{r},\boldsymbol{Q})\frac{\partial\delta(\boldsymbol{Q}-\boldsymbol{Q}')}{\partial \boldsymbol{r}},$$
$$M_{52}=-\chi\dot{\boldsymbol{\gamma}}:\boldsymbol{a}_4,$$
$$M_{25}=-\chi\boldsymbol{a}_4:\dot{\boldsymbol{\gamma}},$$
$$M_{55}\cdot\frac{\partial s_{\mathrm{f}}}{\partial \boldsymbol{a}_2(\boldsymbol{r})}=2D_{\mathrm{r}}(\boldsymbol{I}-m\cdot\boldsymbol{a}_2),$$

其中 e_{f} 和 s_{f} 均与 M_{55} 相关

$$-(\chi\dot{\boldsymbol{\gamma}}:\boldsymbol{a}_4)\cdot\boldsymbol{v}(\boldsymbol{r})+M_{55}\cdot\frac{\partial e_{\mathrm{f}}}{\partial \boldsymbol{a}_2(\boldsymbol{r})}=0.$$

由算子 L 和 M 确定的纤维悬浮聚合物溶液的均一 GENERIC 结构可以得出纤维取向引起的应力贡献 $\boldsymbol{\tau}_{\mathrm{f}}$ 表达式为

$$\boldsymbol{\tau}_{\mathrm{f}}=\frac{\partial}{\partial \boldsymbol{r}}\boldsymbol{\Pi}'(\boldsymbol{r})+L_{25}\frac{\partial e_{\mathrm{f}}}{\partial \boldsymbol{a}_2(\boldsymbol{r})}+M_{25}\frac{\partial s_{\mathrm{f}}}{\partial \boldsymbol{a}_2(\boldsymbol{r})}. \tag{40}$$

4.2. 基于构型张量的均一结构多尺度模型

根据所选聚合物材料的性质,若需要对分子链的列向信息进一步关注,即为了更好地反映单位长度的分子链拉伸和取向程度,可以使用基于大分子哑铃描述中经常使用的〈QQ〉定义的分子链构型张量 $\boldsymbol{c}$,得到从构型张量到应力张量的复杂熔体的 GENERIC 形式多尺度模型. 因此,系统的独立变量可选取为 $x=\{\rho,\boldsymbol{u},\varepsilon,\boldsymbol{c},\boldsymbol{a}_2\}$,其中 $e_{\mathrm{p}}(\rho,\boldsymbol{c})$ 和 $s_{\mathrm{p}}(\rho,\boldsymbol{c})$ 分别表示与聚合物大分子链模型相关的能量贡献和熵贡献,这样总能量 E 和熵 S 可表示为

$$E=\int\Big[\frac{1}{2}\frac{\boldsymbol{u}(\boldsymbol{r})^2}{\rho(\boldsymbol{r})}+\varepsilon(\boldsymbol{r})$$
$$+e_{\mathrm{p}}(\rho,\boldsymbol{c})+e_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)\Big]\mathrm{d}^3r, \tag{41}$$

$$S=\int\Big\{\boldsymbol{s}(\boldsymbol{\rho}(\boldsymbol{r}),\varepsilon(\boldsymbol{r}))+s_{\mathrm{p}}(\rho,\boldsymbol{c})+s_{\mathrm{f}}(\boldsymbol{r},\boldsymbol{a}_2)\Big\}\mathrm{d}^3r. \tag{42}$$

由(41)式,(42)式,可得

$$\frac{\delta E}{\delta x}=\begin{pmatrix}-\frac{1}{2}\boldsymbol{v}(\boldsymbol{r})^2\\ \boldsymbol{v}(\boldsymbol{r})\\ 1\\ \frac{\partial e_p}{\partial \boldsymbol{c}(\boldsymbol{r})}\\ \frac{\partial e_f}{\partial \boldsymbol{a}_2(\boldsymbol{r})}\end{pmatrix}, \tag{43}$$

$$\frac{\delta S}{\delta x}=\begin{pmatrix}-\frac{\mu(\boldsymbol{r})}{T(\boldsymbol{r})}\\ 0\\ \frac{1}{T(\boldsymbol{r})}\\ \frac{\partial s_p}{\partial \boldsymbol{c}(\boldsymbol{r})}\\ \frac{\partial s_f}{\partial \boldsymbol{a}_2(\boldsymbol{r})}\end{pmatrix}. \tag{44}$$

作为逆变变形张量,哑铃构型张量 $\boldsymbol{c}$ 的变换行为如下:

$$\boldsymbol{c}(\boldsymbol{r})\to\boldsymbol{c}(\boldsymbol{r})-t\left\{\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{c}(\boldsymbol{r})]-\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\cdot\boldsymbol{c}(\boldsymbol{r})-\boldsymbol{c}(\boldsymbol{r})\cdot\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]^{\mathrm{T}}\right\}. \tag{45}$$

经由

$$\begin{pmatrix}-\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\rho(\boldsymbol{r})]\\ -\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{u}(\boldsymbol{r})]-\left(\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\cdot\boldsymbol{u}(\boldsymbol{r})\\ -\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\varepsilon(\boldsymbol{r})-[p(\boldsymbol{r})\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r})]:\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\\ -\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{c}(\boldsymbol{r})]+\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\cdot\boldsymbol{c}(\boldsymbol{r})+\boldsymbol{c}(\boldsymbol{r})\cdot\left(\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]^{\mathrm{T}}\\ \left\{-\frac{\partial}{\partial\boldsymbol{r}}\cdot[\boldsymbol{v}(\boldsymbol{r})\boldsymbol{a}_2(\boldsymbol{r})]+\frac{1}{2}(\chi-1)\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]^{\mathrm{T}}\cdot\boldsymbol{a}_2+\frac{1}{2}(\chi+1)\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\cdot\boldsymbol{a}_2\right.\\ \left.+\frac{1}{2}\boldsymbol{a}_2\cdot(\chi+1)\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]^{\mathrm{T}}+\frac{1}{2}\boldsymbol{a}_2\cdot(\chi-1)\left[\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{v}(\boldsymbol{r})\right]\right\}\end{pmatrix}=\int L(\boldsymbol{r},\boldsymbol{r}')\cdot\begin{pmatrix}\frac{\delta G}{\delta\rho(\boldsymbol{r}')}\\ \frac{\delta G}{\delta\boldsymbol{u}(\boldsymbol{r}')}\\ \frac{\delta G}{\delta\varepsilon(\boldsymbol{r}')}\\ \frac{\delta G}{\delta\boldsymbol{c}(\boldsymbol{r}')}\\ \frac{\delta G}{\delta\boldsymbol{a}_2(\boldsymbol{r}')}\end{pmatrix}\mathrm{d}^3\boldsymbol{r}',$$

可得

$$L(\boldsymbol{r},\boldsymbol{r}')=\begin{pmatrix}0 & \rho(\boldsymbol{r}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'} & 0 & 0 & 0\\ \rho(\boldsymbol{r})\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'} & \begin{matrix}\boldsymbol{u}(\boldsymbol{r}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{u}(\boldsymbol{r})\end{matrix} & \begin{matrix}\varepsilon(\boldsymbol{r})\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ \cdot[p(\boldsymbol{r}')\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r}')]\end{matrix} & L_{24} & L_{25}\\ 0 & \begin{matrix}\varepsilon(\boldsymbol{r}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ +\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\\ \cdot[p(\boldsymbol{r})\boldsymbol{I}+\boldsymbol{\Pi}(\boldsymbol{r})]\end{matrix} & 0 & 0 & 0\\ 0 & L_{42} & 0 & 0 & 0\\ 0 & L_{52} & 0 & 0 & 0\end{pmatrix},$$

$$L_{24}=\boldsymbol{c}(\boldsymbol{r})\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{c}(\boldsymbol{r}')-\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{c}(\boldsymbol{r}'),$$

$$L_{25}=\boldsymbol{a}_2(\boldsymbol{r})\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{a}_2(\boldsymbol{r}')$$
$$-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}')-\frac{1}{2}(\chi-1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}'),$$

$$L_{42}=\boldsymbol{c}(\boldsymbol{r}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{c}(\boldsymbol{r})-\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{c}(\boldsymbol{r}),$$

$$\begin{aligned}L_{52}=&\boldsymbol{a}_2(\boldsymbol{r}')\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r}')\cdot\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\boldsymbol{a}_2(\boldsymbol{r})\\&-\frac{1}{2}(\chi+1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r})-\frac{1}{2}(\chi-1)\frac{\partial\delta(\boldsymbol{r}-\boldsymbol{r}')}{\partial\boldsymbol{r}'}\cdot\boldsymbol{a}_2(\boldsymbol{r}).\end{aligned}$$

为满足 $L\frac{\delta S}{\delta x}=0$，$\boldsymbol{\Pi}(\boldsymbol{r})=-2\boldsymbol{c}\cdot z+\boldsymbol{\Pi}'(\boldsymbol{r})=2\boldsymbol{c}\cdot T\frac{\partial s_{\mathrm{p}}}{\partial\boldsymbol{c}}+\boldsymbol{\Pi}'(\boldsymbol{r})$，其中 $\boldsymbol{\Pi}'(\boldsymbol{r})$仍满足(38)式.

经 r' 上的积分后，有

$$L(\boldsymbol{r})=-\begin{pmatrix}0 & \frac{\partial\delta}{\partial\boldsymbol{r}}\rho(\boldsymbol{r}) & 0 & 0 & 0\\ \rho(\boldsymbol{r})\frac{\partial\delta}{\partial\boldsymbol{r}} & \left[\frac{\partial\delta}{\partial\boldsymbol{r}}\boldsymbol{u}(\boldsymbol{r})+\boldsymbol{u}(\boldsymbol{r})\frac{\partial\delta}{\partial\boldsymbol{r}}\right]^{\mathrm{T}} & \begin{gathered}\varepsilon(\boldsymbol{r})\frac{\partial}{\partial\boldsymbol{r}}\\+\frac{\partial}{\partial\boldsymbol{r}}p(\boldsymbol{r})+\frac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{\Pi}(\boldsymbol{r})\end{gathered} & L_{24} & L_{25}\\ 0 & \begin{gathered}\frac{\partial}{\partial\boldsymbol{r}}\varepsilon(\boldsymbol{r})+p(\boldsymbol{r})\frac{\partial}{\partial\boldsymbol{r}}\\+\boldsymbol{\Pi}(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}}\end{gathered} & 0 & 0 & 0\\ 0 & L_{42} & 0 & 0 & 0\\ 0 & L_{52} & 0 & 0 & 0\end{pmatrix},\tag{46}$$

$$L_{24}=\boldsymbol{c}(\boldsymbol{r})\frac{\partial}{\partial\boldsymbol{r}}-\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{c}(\boldsymbol{r})-\frac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{c}(\boldsymbol{r}),$$

$$\begin{aligned}L_{25}=&\boldsymbol{a}_2(\boldsymbol{r})\frac{\partial}{\partial\boldsymbol{r}}-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}}\\&-\frac{1}{2}(\chi+1)\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{a}_2(\boldsymbol{r})\\&-\frac{1}{2}(\chi+1)\frac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{a}_2(\boldsymbol{r})\\&-\frac{1}{2}(\chi-1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}},\end{aligned}$$

$$L_{42}=\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{c}(\boldsymbol{r})-\boldsymbol{c}(\boldsymbol{r})\frac{\partial}{\partial\boldsymbol{r}}-\boldsymbol{c}(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}},$$

$$\begin{aligned}L_{52}=&\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{a}_2(\boldsymbol{r})-\frac{1}{2}(\chi-1)\frac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{a}_2(\boldsymbol{r})\\&-\frac{1}{2}(\chi+1)\frac{\partial}{\partial\boldsymbol{r}}\boldsymbol{a}_2(\boldsymbol{r})-\frac{1}{2}(\chi+1)\boldsymbol{a}_2(\boldsymbol{r})\cdot\frac{\partial}{\partial\boldsymbol{r}}\\&-\frac{1}{2}(\chi-1)\frac{\partial}{\partial\boldsymbol{r}}\cdot\boldsymbol{a}_2(\boldsymbol{r}).\end{aligned}$$

$-\boldsymbol{\Lambda}z$ 可看作与哑铃构型张量 $\boldsymbol{c}$ 相关的聚合物溶液的扩散行为，其中 $\boldsymbol{\Lambda}$ 为反映松弛效应的迁移率张量. 结合纤维的扩散行为，可得到与 e_{p}，e_{f}，s_{p}，s_{f} 表达式相关的度量矩阵 M，

$$M(\boldsymbol{r})=\begin{pmatrix}0 & 0 & 0 & 0 & 0\\ 0 & -\left(\frac{\partial}{\partial\boldsymbol{r}}\eta_{\mathrm{s}}T\frac{\partial}{\partial\boldsymbol{r}}\right)^{\mathrm{T}}-\boldsymbol{I}\frac{\partial}{\partial\boldsymbol{r}}\cdot\eta_{\mathrm{s}}T\frac{\partial}{\partial\boldsymbol{r}} & \frac{\partial}{\partial\boldsymbol{r}}\cdot\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}} & 0 & M_{25}\\ 0 & -\eta_{\mathrm{s}}T\bar{\dot{\boldsymbol{\gamma}}}\frac{\partial}{\partial\boldsymbol{r}} & M_{33} & M_{34} & 0\\ 0 & 0 & M_{43} & M_{44} & 0\\ 0 & M_{52} & 0 & 0 & M_{55}\end{pmatrix},\tag{47}$$

$$\begin{aligned}M_{33}=&\frac{1}{2}\eta_{\mathrm{s}}T\dot{\boldsymbol{\gamma}}:\dot{\boldsymbol{\gamma}}-\frac{\partial}{\partial\boldsymbol{r}}\cdot k_{\mathrm{p}}T^2\frac{\partial}{\partial\boldsymbol{r}}\\&+T\frac{\partial e_{\mathrm{p}}}{\partial\boldsymbol{c}}\cdot\boldsymbol{\Lambda}\cdot\frac{\partial e_{\mathrm{p}}}{\partial\boldsymbol{c}},\end{aligned}$$

$$M_{34}=-T\frac{\partial e_{\mathrm{p}}}{\partial\boldsymbol{c}}\boldsymbol{\Lambda},$$

$$M_{43}=-T\boldsymbol{\Lambda}\frac{\partial e_{\mathrm{p}}}{\partial\boldsymbol{c}},$$

$$M_{44} = T\boldsymbol{\Lambda},$$
$$M_{52} = -\chi\dot{\boldsymbol{\gamma}} : \boldsymbol{a}_4,$$
$$M_{25} = -\chi\boldsymbol{a}_4 : \dot{\boldsymbol{\gamma}},$$
$$M_{55}\cdot\frac{\partial s_{\mathrm{f}}}{\partial \boldsymbol{a}_2(\boldsymbol{r})} = 2D_{\mathrm{r}}(\boldsymbol{I} - m\cdot\boldsymbol{a}_2),$$

为了表征纤维与聚合物溶液的关联性，根据文献[10]，迁移率张量可写为

$$\Lambda_{ijkl} = \Lambda_0[\alpha_1(\boldsymbol{c}_{ij}\boldsymbol{I}_{jk} + \boldsymbol{c}_{ik}\boldsymbol{I}_{jl} + \boldsymbol{I}_{il}\boldsymbol{c}_{jk} + \boldsymbol{I}_{ik}\boldsymbol{c}_{jl}) + \alpha_2(\boldsymbol{c}_{il}a_{jk} + a_{ik}\boldsymbol{c}_{jl})], \tag{48}$$

其中最后一项考虑了纤维与聚合物基体溶液的相互作用．Λ_0 是现象参数，与所选不同的大分子链模型相关，如对于 Maxwell 和 OB 模型[11]，Λ_0 可表示为 $1/(2\rho\alpha\lambda H)$（这里 α 为单位质量溶液内弹性程度的度量，λ 是黏弹性系统的松弛时间），对于 FENE 模型[10]，一般取 0.05，0.001，0.0001 或 0.005 即可．α_1，α_2 是关于纤维浓度和特征的常数，若 $\alpha_2 = 0$，则表示不考虑纤维与聚合物之间的相互作用．

5. 结　论

本文针对处于非平衡态的非等温纤维悬浮聚合物溶液，建立了具有均一 GENERIC 结构的多尺度模型方程组．在该结构的多尺度模型方程组中，根据不同的聚合物大分子链本构模型以及纤维与大分子链间的不同耦合关联，可以进行多尺度模型方程的结构分量调整，而不影响整个复杂系统多尺度模型的均一结构．通过该均一结构的多尺度模型方程组还可以得到系统不同尺度上的应力贡献，进而为系统多尺度间的信息提供更佳的关联耦合．

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A multi-scale model with GENERIC structure of polymeric melt with fiber suspensions*

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Abstract

Based on elastic dumbbell model of polymer melt and tensor description of fiber orientation, a mathematic multi-scale model with a general equation for the non-equilibrium reversible-irreversible coupling (GENERIC) of polymeric melt with fiber suspensions is presented by the coupling of reversible and irreversible thermodynamics. And the model provides a general framework with homogeneous GENERIC structure for the multi-scale governing equations. Through analyzing the components of GENERIC structure, stress contributions from information on different scales can be achieved.

Keywords: GENERIC structure, fiber orientation, viscoelasticity, polymer

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