

VVPF

Documentation for VVPF 2.0 and 3.x

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Contents

1	Microstructural material model	2
1.1	Proposed material model	2
2	Computational Rheology	3
2.1	The Constitutive Equation [pp.16-20]	3
2.2	Velocity Profile [p.56; p.155; pp.391-392]	3
2.3	Shear Stress	4
2.4	Numerical Governing Equation	4
2.5	Shear Rate	6
3	Numerical Results	7
3.1	Power of the Forces \mathbf{t} and $\rho \mathbf{g}$ [pp.389-390]	7

Introduction

This is a working manual for the VVPF software. The document is in its infancy, so there is still a lot of work left. In its current state, this manual is practical useless. This is something I hope to change in the future.

The current report is about the VVPF as well as on the PFI-theory.

Chapters 1 to 3 are based on, and taken from the following Ph.D. thesis:

J. E. Wallevik, Rheology of Particle Suspensions; Fresh Concrete, Mortar and Cement Paste with Various Types of Lignosulfonates, Ph.D. thesis, Department of Structural Engineering, The Norwegian University of Science and Technology, Trondheim, 2003 (ISBN 82-471-5566-4; ISSN 0809-103X). <http://publications.uu.se/ntnu/theses/abstract.xsql?dbid=319>

A reference number in this report designates the corresponding page number of the Ph.D. thesis. I am just using it now as a basis. In the future version of this documentation, I will rather make a reference where appropriate to the above phd thesis.

Chapter 1

Microstructural material model

1.1 Proposed material model

Here, the perikinetic coagulation rate theory, established by Verwey and Overbeek is employed [?]. In their calculation, the decreasing number of particles n_t (in the suspension) is expressed as follows:

$$-\frac{dn_t}{dt} = \frac{H n_t^2}{n_3} \quad (\dot{\gamma} = 0) \quad (1.1)$$

The previous work done by Hattori and Izumi and used in this article, consists of the following three equations [?]:

$$\eta \propto U_3^{2/3} \quad (1.2)$$

$$n_t = n_3 - J_t \quad (1.3)$$

$$J_t = n_3 U_3 \quad (1.4)$$

$$-\frac{dn_t}{dt} = -\frac{d(n_3 - J_t)}{dt} = \frac{dJ_t}{dt} = n_3 \frac{dU_3}{dt} \quad (1.5)$$

$$n_3 \frac{dU_3}{dt} = H \frac{(n_3 - J_t)^2}{n_3} = H \frac{n_3^2(1 - U_3)^2}{n_3} \quad (1.6)$$

$$n_3 \frac{dU_3}{dt} = H(\dot{\gamma}, t, \dots) \frac{n_3^2(1 - U_3)^2}{n_3} + f_1(I(\dot{\gamma}, t, \dots), \dot{\gamma}) \quad (1.7)$$

$$\frac{dU_3}{dt} = H(\dot{\gamma}, t, \dots) (1 - U_3)^2 + f_2(I(\dot{\gamma}, t, \dots), \dot{\gamma}) \quad (1.8)$$

$$\frac{dU_3}{dt} = f(U_3, H, I, \dot{\gamma}, d\dot{\gamma}/dt, t, \dots) \quad \wedge \quad U_3 = U_o \quad \text{at} \quad t = 0 \quad (1.9)$$

$$\tilde{\mu} = \xi_1 U_3^{2/3} \quad (1.10)$$

$$\tilde{\tau}_o = \xi_2 U_3^{2/3} \quad (1.11)$$

Although determined by empirical means in this work, the two terms ξ_1 and ξ_2 are material parameters depending, among other factors, on the surface roughness of the cement particles and phase volume Φ .

$$\eta = \left(\mu + \frac{\tau_o}{\dot{\gamma}} \right) + \left(\tilde{\mu} + \frac{\tilde{\tau}_o}{\dot{\gamma}} \right) \quad (1.12)$$

Chapter 2

Computational Rheology

2.1 The Constitutive Equation [pp.16-20]

For many fluids, the constitutive equation is represented as $\boldsymbol{\sigma} = -p\mathbf{I} + \mathbf{T}$, where the second order tensor $\mathbf{T} = T_{ij}\mathbf{i}_i\mathbf{i}_j$ is known as the **extra stress tensor** and p is the pressure. The term \mathbf{I} , is known as the **unit dyadic** and its index equivalence is the **Kronecker delta**, written as δ_{ij} where $\delta_{ij} = 1$ if $i = j$ and $\delta_{ij} = 0$ if $i \neq j$. In index notation, the tensor $\boldsymbol{\sigma}$ is written as: $\sigma_{ij} = -p\delta_{ij} + T_{ij}$. According to customary understanding, σ_{ij} designates a stress in j -direction on a plane that has a normal unit vector pointing in i -direction. Furthermore, it can be shown that this tensor is symmetric: $\sigma_{ij} = \sigma_{ji}$. The same considerations applies for T_{ij} . In [pp.21-28], this tensor is associated with the exchange of momentum between solid particles of the continuum.

The constitutive equation used in this report has the following functional form [p.17]:

$$\boldsymbol{\sigma}(\mathbf{x}, t) = -p(\mathbf{x}, t)\mathbf{I} + \mathbf{T}(\mathbf{x}, t) \quad \wedge \quad \mathbf{T}(\mathbf{x}, t) = 2\eta(\mathbf{x}, t)\dot{\boldsymbol{\epsilon}}(\mathbf{x}, t) \quad (2.1)$$

where p is the pressure and η is the shear viscosity. Example of a shear viscosity equation is of the Bingham fluid $\eta = \mu + \tau_o/\dot{\gamma}$. As will be clear later in this report, no specific shear viscosity equation is assumed in the analysis. It can be of any type, with or without time-dependence.

The tensor $\dot{\boldsymbol{\epsilon}} = \dot{\epsilon}_{ij}\mathbf{i}_i\mathbf{i}_j$ is called the **strain rate tensor** and is given by [See p.17]:

$$\dot{\boldsymbol{\epsilon}} = \frac{1}{2}(\nabla\mathbf{v} + (\nabla\mathbf{v})^T) = \frac{1}{2}\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right)\mathbf{i}_i\mathbf{i}_j \quad (2.2)$$

In the last part of the above, a so-called *indicial notation* in Cartesian coordinate system, is used. The velocity gradient tensor $\nabla\mathbf{v} = [\partial v_i/\partial x_j]\mathbf{i}_i\mathbf{i}_j$ can be looked upon as a comparison of velocities between CPs, placed around the CP in question. With CP, it is meant continuum particle (or *fluid particle*) [see pp.11-16 about the CP]. The term $\dot{\gamma}$ is known as the shear rate and is a function of the strain rate tensor as shown with Equation 2.3 [p.24].

$$\dot{\gamma} = \sqrt{2\dot{\boldsymbol{\epsilon}} : \dot{\boldsymbol{\epsilon}}} = \sqrt{2\dot{\epsilon}_{ij}\dot{\epsilon}_{ij}} \quad (2.3)$$

The governing equation (i.e. Newton's second law for the CP) is [pp.11-16]:

$$\rho(\mathbf{x}, t) \left(\frac{\partial \mathbf{v}(\mathbf{x}, t)}{\partial t} + \mathbf{v}(\mathbf{x}, t) \cdot \nabla \mathbf{v}(\mathbf{x}, t) \right) = \nabla \cdot \boldsymbol{\sigma}(\mathbf{x}, t) + \rho(\mathbf{x}, t) \mathbf{g} \quad (2.4)$$

2.2 Velocity Profile [p.56; p.155; pp.391-392]

Because of convenience, the cylindrical coordinates will be used here. By using the general velocity field $\mathbf{v} = v_r(r, \theta, z, t)\mathbf{i}_r + v_\theta(r, \theta, z, t)\mathbf{i}_\theta + v_z(r, \theta, z, t)\mathbf{i}_z$ it is impossible to gain an analytical solution. But fortunately some reasonable assumptions about the flow can be made, which makes it easier to obtain such a solution:

1. With low Reynolds number (i.e. with low speed and high shear viscosity η) the flow is stable¹ and it is possible to assume a flow symmetry around the z -axis: $\mathbf{v} = v_r(r, \theta, z, t)\mathbf{i}_r + v_\theta(r, \theta, z, t)\mathbf{i}_\theta$.

¹As random motion (Brownian motion) of water molecules (in water) is not understood as *fluid mechanical* turbulence, then neither are the random and spontaneous velocity contributions of individual solid particles (in suspension) understood as such. Rather, when groups of continuum particles (CPs), inside the continuum, start to travel coherently in circular paths, as a part of eddies or vortices of varying size, it is possible to define turbulence. More precisely, turbulent flow is characterized by a mixing action caused by eddies of varying size, throughout the continuum [see citation Roberson in PhD thesis].

2. With the lower unit of the inner cylinder (see Figure 3.4), the effect of shearing from the bottom plate is eliminated. Therefore a height independence can be assumed in the velocity function: $\mathbf{v} = v_r(r, \theta, t) \mathbf{i}_r + v_\theta(r, \theta, t) \mathbf{i}_\theta$. For both CONTEC viscometers, this assumption is verified by numerical means in ChapterPhD 8 (see FigPhD 8.16, Page 197 and FigPhD 8.21, Page 200).
3. Due to the circular geometry of a coaxial cylinders viscometer (see FigPhD 3.1) it is reasonable to assume pure circular flow with θ -independence.

$$\mathbf{v} = v_\theta(r, t) \mathbf{i}_\theta \quad (2.5)$$

A physical description of velocity \mathbf{v} is given by EqPhD 2.6 on Page 13 (see also the discussion below EqPhD 2.6).

From here on, it is assumed that the outer cylinder rotates counterclockwise, giving $v_\theta(r, t) \geq 0$. This is done to simplify the calculations that follow. For both CONTEC viscometers involved, the outer cylinder actually rotates clockwise. Nevertheless, the calculations apply fully for either clockwise or counterclockwise rotating outer cylinder.

2.3 Shear Stress

From Equation 2.5 the velocity gradient tensor $\nabla \mathbf{v}$ can be calculated, which through Equation 2.2, gives the strain rate tensor:

$$\dot{\boldsymbol{\varepsilon}} = \frac{1}{2} \left(\frac{\partial v_\theta(r, t)}{\partial r} - \frac{v_\theta(r, t)}{r} \right) (\mathbf{i}_r \mathbf{i}_\theta + \mathbf{i}_\theta \mathbf{i}_r) \quad (2.6)$$

Substituting the result from Equation 2.6 into Equation 2.3 gives the shear rate that applies inside the test material.

$$\dot{\gamma} = \left| \frac{\partial v_\theta(r, t)}{\partial r} - \frac{v_\theta(r, t)}{r} \right| \quad (2.7)$$

c.f. SectionPhD 3.3.3, Page 58 (i.e. from a physical point of view, then $\tau(r, t) \geq 0$ and $\eta(r, t) \geq 0$ in Eq. (2.8)). Combining Equations 2.1 and 2.6, yields the extra stress tensor:

$$\mathbf{T} = \eta(r, t) \left(\frac{\partial v_\theta(r, t)}{\partial r} - \frac{v_\theta(r, t)}{r} \right) (\mathbf{i}_r \mathbf{i}_\theta + \mathbf{i}_\theta \mathbf{i}_r) = \tau(r, t) (\mathbf{i}_r \mathbf{i}_\theta + \mathbf{i}_\theta \mathbf{i}_r) \quad (2.8)$$

Although the shear viscosity $\eta = \eta(\dot{\gamma}, t, \dots)$ is dependent on various of variables, the basic independent variables are r and t , i.e. $\eta = \eta(r, t)$. The term $\tau(r, t)$ is now extracted directly from Equation 2.8:

$$\tau(r, t) = \eta(r, t) \left(\frac{\partial v_\theta(r, t)}{\partial r} - \frac{v_\theta(r, t)}{r} \right) \Rightarrow \tau_i = \eta_i \left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r} \right]_i \quad (2.9)$$

C.f. Eq. (2.7).

The von Mises shear stress is $\tau^2 = -\Pi_{\mathbf{S}}^{\text{P}} = (\mathbf{T} : \mathbf{T})/2 = (2\eta)^2 \dot{\boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}}/2 = \eta^2 (2\dot{\boldsymbol{\varepsilon}} : \dot{\boldsymbol{\varepsilon}}) = (\eta\dot{\gamma})^2$.

2.4 Numerical Governing Equation

Using the velocity profile Eq. (2.5) in Eqs. (2.1), (2.4) and (2.8) gives:

$$\rho \frac{\partial v_\theta(r, t)}{\partial t} = \frac{\partial \tau(r, t)}{\partial r} + 2 \frac{\tau(r, t)}{r} \quad (2.10)$$

The term $\tau(r, t)$ is given by Eq. 2.9. The above equation applies in the θ -direction. In this derivation, two other equations are also produced: $0 = -\partial p(r, z, t)/\partial z - \rho g$ and $-\rho v_\theta^2(r, t)/r = -\partial p(r, z, t)/\partial r$. These apply in z - and r -directions, respectively. Fortunately, they are not directly coupled to Equation 2.10 and hence need not to be included in the numerical simulation.

When discretizing the governing Equation ?? one might be tempted to put Equation ?? in this equation and then expanding the velocity terms, for examples from $\partial(\eta v)/\partial r$ to $v \partial \eta/\partial r + \eta \partial^2 v/\partial r^2$ and so forth. According to Langtangen then such a procedure should be avoided [?]. Therefore a discretization of Equation ?? as it is, will be done.

In discretizing the governing Equation ?? a centered differencing in space will be used. This is done to increase accuracy from $O(\Delta r)$ to $O(\Delta r)^2$ [?]. Also, an implicit scheme (see for example [?]) will be used in the time stepping to increase stability in the numerical calculations.

$$\rho \frac{v_i^{k+1} - v_i^k}{\Delta t} = \frac{\tau_{i+\frac{1}{2}}^{k+1} - \tau_{i-\frac{1}{2}}^{k+1}}{\Delta r} + 2 \frac{\tau_i^{k+1}}{r_i} \quad (2.11)$$

$$v_i^{k+1} - v_i^k = \beta(\tau_{i+\frac{1}{2}}^{k+1} - \tau_{i-\frac{1}{2}}^{k+1}) + \theta_i \tau_i^{k+1} \quad (2.12)$$

where $\beta = \Delta t / (\rho \Delta r)$ and $\theta_i = (2 \Delta t) / (\rho r_i)$.

$$\begin{aligned} \left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r} \right]_i &= \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{\Delta r} - \frac{v_i}{r_i} = \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{\Delta r} - \frac{(v_{i+\frac{1}{2}} + v_{i-\frac{1}{2}})/2}{(r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}})/2} \\ &= \left[\frac{1}{\Delta r} - \frac{1}{r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}}} \right] v_{i+\frac{1}{2}} - \left[\frac{1}{\Delta r} + \frac{1}{r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}}} \right] v_{i-\frac{1}{2}} \end{aligned} \quad (2.13)$$

$$\left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r} \right]_{i+\frac{1}{2}} = \left[\frac{1}{\Delta r} - \frac{1}{r_{i+1} + r_i} \right] v_{i+1} - \left[\frac{1}{\Delta r} + \frac{1}{r_{i+1} + r_i} \right] v_i \quad (2.14)$$

$$\left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r} \right]_{i-\frac{1}{2}} = \left[\frac{1}{\Delta r} - \frac{1}{r_i + r_{i-1}} \right] v_i - \left[\frac{1}{\Delta r} + \frac{1}{r_i + r_{i-1}} \right] v_{i-1} \quad (2.15)$$

$$\begin{aligned} \left[\frac{\partial v_\theta}{\partial r} - \frac{v_\theta}{r} \right]_i &= \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{\Delta r} - \frac{v_i}{r_i} = \frac{\frac{1}{2}(v_{i+1} + v_i) - \frac{1}{2}(v_i + v_{i-1})}{\Delta r} - \frac{v_i}{r_i} \\ &= \frac{v_{i+1} - v_{i-1}}{2 \Delta r} - \frac{v_i}{r_i} \end{aligned} \quad (2.16)$$

$$\begin{aligned} \tau_{i+\frac{1}{2}} &= \left(\eta_{i+\frac{1}{2}} \left[\frac{1}{\Delta r} - \frac{1}{r_{i+1} + r_i} \right] \right) v_{i+1} - \left(\eta_{i+\frac{1}{2}} \left[\frac{1}{\Delta r} + \frac{1}{r_{i+1} + r_i} \right] \right) v_i \\ &= \Xi_{i+1} v_{i+1} - \Theta_{i+1} v_i \end{aligned} \quad (2.17)$$

$$\begin{aligned} \tau_i &= \eta_i \frac{v_{i+1} - v_{i-1}}{2 \Delta r} - \eta_i \frac{v_i}{r_i} = \left(\frac{\eta_i}{2 \Delta r} \right) v_{i+1} - \left(\frac{\eta_i}{r_i} \right) v_i - \left(\frac{\eta_i}{2 \Delta r} \right) v_{i-1} \\ &= \Psi_i v_{i+1} - \Lambda_i v_i - \Psi_i v_{i-1} \end{aligned} \quad (2.18)$$

$$\begin{aligned} \tau_{i-\frac{1}{2}} &= \left(\eta_{i-\frac{1}{2}} \left[\frac{1}{\Delta r} - \frac{1}{r_i + r_{i-1}} \right] \right) v_i - \left(\eta_{i-\frac{1}{2}} \left[\frac{1}{\Delta r} + \frac{1}{r_i + r_{i-1}} \right] \right) v_{i-1} \\ &= \Xi_i v_i - \Theta_i v_{i-1} \end{aligned} \quad (2.19)$$

$$\begin{aligned} v_i^{k+1} - v_i^k &= \beta [\Xi_{i+1}^{k+1} v_{i+1}^{k+1} - \Theta_{i+1}^{k+1} v_i^{k+1} - \Xi_i^{k+1} v_i^{k+1} + \Theta_i^{k+1} v_{i-1}^{k+1}] + \\ &\quad + \theta_i [\Psi_i^{k+1} v_{i+1}^{k+1} - \Lambda_i^{k+1} v_i^{k+1} - \Psi_i^{k+1} v_{i-1}^{k+1}] \end{aligned} \quad (2.20)$$

$$\begin{aligned} v_i^{k+1} - v_i^k &= [\beta \Xi_{i+1}^{k+1} + \theta_i \Psi_i^{k+1}] v_{i+1}^{k+1} - [\beta \Theta_{i+1}^{k+1} + \beta \Xi_i^{k+1} + \theta_i \Lambda_i^{k+1}] v_i^{k+1} + \\ &\quad + [\beta \Theta_i^{k+1} - \theta_i \Psi_i^{k+1}] v_{i-1}^{k+1} \end{aligned} \quad (2.21)$$

$$v_i^{k+1} - v_i^k = A_i^{k+1} v_{i+1}^{k+1} - B_i^{k+1} v_i^{k+1} + C_i^{k+1} v_{i-1}^{k+1} \quad (2.22)$$

$$A_i^{k+1} v_{i+1}^{k+1} - (1 + B_i^{k+1}) v_i^{k+1} + C_i^{k+1} v_{i-1}^{k+1} = -v_i^k \quad (2.23)$$

$$A_i^{k+1} = \beta \Xi_{i+1}^{k+1} + \theta_i \Psi_i^{k+1} = \beta \eta_{i+\frac{1}{2}}^{k+1} \left[\frac{1}{\Delta r} - \frac{1}{r_{i+1} + r_i} \right] + \theta_i \frac{\eta_i^{k+1}}{2 \Delta r} \quad (2.24)$$

$$\begin{aligned} B_i^{k+1} &= \beta \Theta_{i+1}^{k+1} + \beta \Xi_i^{k+1} + \theta_i \Lambda_i^{k+1} = \\ &= \beta \eta_{i+\frac{1}{2}}^{k+1} \left[\frac{1}{\Delta r} + \frac{1}{r_{i+1} + r_i} \right] + \beta \eta_{i-\frac{1}{2}}^{k+1} \left[\frac{1}{\Delta r} - \frac{1}{r_i + r_{i-1}} \right] + \theta_i \frac{\eta_i^{k+1}}{r_i} \end{aligned} \quad (2.25)$$

$$C_i^{k+1} = \beta \Theta_i^{k+1} - \theta_i \Psi_i^{k+1} = \beta \eta_{i-\frac{1}{2}}^{k+1} \left[\frac{1}{\Delta r} + \frac{1}{r_i + r_{i-1}} \right] - \theta_i \frac{\eta_i^{k+1}}{2 \Delta r} \quad (2.26)$$

From Eq. (1.9) we have

$$\frac{dU_3}{dt} = f(U_3, H, I, \dot{\gamma}, d\dot{\gamma}/dt, t, \dots) \quad \wedge \quad U_3 = U_o \quad \text{at} \quad t = 0 \quad (2.27)$$

$$\frac{U_{3,i}^{k+1} - U_{3,i}^k}{\Delta t} = f(U_{3,i}^{k+1}, H_i^{k+1}, I_i^{k+1}, \dot{\gamma}_i^{k+1}, d\dot{\gamma}_i^{k+1}/dt, t, \dots) \quad \wedge \quad U_3 = U_o \quad \text{at} \quad t = 0 \quad (2.28)$$

2.5 Shear Rate

It is apparent that information about the shear viscosity η at the grid points $(i+\frac{1}{2})$ and $(i-\frac{1}{2})$ is needed. Since $\eta_i = \eta(\dot{\gamma}_i, \tilde{\Gamma}_i, \tilde{\Theta}_i, k \Delta t)$, one must first calculate the shear rate $\dot{\gamma}_i$ at the corresponding points.

$$\dot{\gamma} = \left| \frac{\partial v_\theta(r, t)}{\partial r} - \frac{v_\theta(r, t)}{r} \right| \quad (2.29)$$

$$\dot{\gamma}_i = \left| \frac{v_{i+1} - v_{i-1}}{2 \Delta r} - \frac{v_i}{r_i} \right| \quad (2.30)$$

$$\begin{aligned} \dot{\gamma}_i &= \left| \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{\Delta r} - \frac{v_i}{r_i} \right| = \left| \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{\Delta r} - \frac{(v_{i+\frac{1}{2}} + v_{i-\frac{1}{2}})/2}{(r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}})/2} \right| \\ &= \left| \frac{v_{i+\frac{1}{2}} - v_{i-\frac{1}{2}}}{\Delta r} - \frac{v_{i+\frac{1}{2}} + v_{i-\frac{1}{2}}}{r_{i+\frac{1}{2}} + r_{i-\frac{1}{2}}} \right| \end{aligned} \quad (2.31)$$

$$\dot{\gamma}_{i+\frac{1}{2}} = \left| \frac{v_{i+1} - v_i}{\Delta r} - \frac{v_{i+1} + v_i}{r_{i+1} + r_i} \right| \quad (2.32)$$

$$\dot{\gamma}_{i-\frac{1}{2}} = \left| \frac{v_i - v_{i-1}}{\Delta r} - \frac{v_i + v_{i-1}}{r_i + r_{i-1}} \right| \quad (2.33)$$

Chapter 3

Numerical Results

3.1 Power of the Forces \mathbf{t} and $\rho \mathbf{g}$ [pp.389-390]

The rate in mechanical effort (or rate of work) conducted on the material volume $V(t)$, from its surroundings, is designated with \dot{W} [J/s] and is given by Equation x. The term $\mathbf{g} \cdot \mathbf{v}$ expresses the rate of gravitational work done on the CP. The term¹ $\mathbf{t} \cdot \mathbf{v}$ represents the (viscous) rate of work applied on the CP, from its surroundings.

¹ $\mathbf{t} \cdot \mathbf{v} = (\mathbf{n} \cdot \boldsymbol{\sigma}) \cdot \mathbf{v} = (\boldsymbol{\sigma} \cdot \mathbf{v}) \cdot \mathbf{n}$.