LC-7110

Tieteellinen kirjoittaminen tohtoriopiskelijoille

Aalto-yliopisto
Aalto-universitetet
Aalto University

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- Tekstin rakenne
- Kurssitavoitteet ja tekstipaja 3

Tekstipaja 3

- **Mycoursesissa** tarkempi ohjeistus
- **Lyhyesti:** tutkimustekstiä tai populääriä tekstiä, yksi pidempi tai muutaman yhdistelmä, yht. **4–5 s.**
- **Palautus:** hyvissä ajoin. Pe 26.5. mennessä

Pienryhmissä:

1. Millaisen tekstin aiot tuoda Tekstipaja 3:een?
2. Miksi? Ts. mitä erityisesti toivot oppivasi?
3. Onko sinulla jokin kysymys tai pulma tekstiin liittyen?

Kun olette valmiita:

1. Mikä oli viikkotavoitteesi? Miten se toteutui?
2. Miltä näyttää 11 viikon suunnitelmasi? Onko kevään työskentely mennyt odotetusti vai onko tullut suurempia muutoksia?

Tekstin rakenne: yleistä

Rakenne: yleistä (1)

Kaksi reittiä hyvän rakenteen määrittelyyn

- pihvi: tutkimuksen toteutus, tulokset ja näiden raportointi
- tieteellisen journaalin / toimitetun kirjan tyyliohje.

Tekstin keskeiset ulottuvuudet (rakenteen kannalta)

- Esitystapa (painotus): formaali esitys ↔ luonnollinen kieli
- Suhde tutkimukseen (painotus): raportointi ↔ itse analyysi

Rakenne: yleistä (2)

1. Mitä tullaan tekemään / mitä tehtiin (ylimalkaisesti)

(2. Mahdollisesti lisätaustaa sille, mitä tullaan tekemään)

2. Mitä tehdään / mitä tehtiin (yksityiskohtaisesti)

3. Mitä saatiin aikaiseksi tai tulokseksi

4. Mitä aikaansaannoksista tai tuloksista pitäisi ajatella

5. Mitä tehtiin ja/tai mitä pitäisi tehdä seuraavaksi

Rakenne: yleistä (2)

1. **Introduction.** Mitä tullaan tekemään / mitä tehtiin (ylimalkaisesti)

(2. Background. [tjsp.] lisätaustaa sille, mitä tullaan tekemään)

2. **Materials & methods.** Mitä tehdään / mitä tehtiin (yksityiskohtaisesti)
3. **Results.** Mitä saatiin aikaiseksi tai tulokseksi
4. **Discussion.** Mitä aikaansaannoksista tai tuloksista pitäisi ajatella
5. **Conclusion.** Mitä tehtiin ja/tai mitä pitäisi tehdä seuraavaksi

= IMRAD

Rakenne: yleistä (3)

Rakenteen variaatio tapahtuu keskellä*

- Tutkimusala ja –tyyppi määrittelevät, miten tekstissä painottuvat em. ulottuvuudet (formaali ↔ kielellinen, raportoiva ↔ analysoiva)
- Painotukset määrittelevät artikkelin keskivaiheen sisällöt ja ilmaisutavat
- Sisällöt ja ilmaisutavat (ml. tekstin silkka määrä) määrittelevät miten teksti jaotellaan/kannattaa jaotella
- Käytännön vinkki: lue maalijournaalin artikkeleita tekstirakenne edellä!

*Kun tekstilaji vakioitu. Myös johdannossa ja päätännässä esiintyy tekstinosan *sisäistä variaatiota.*

Tekstin rakenne: ei-niin-yleistä

Keskivaiheen jäsennys

Kemian tekniikka

<u>2 Model description and Filtering procedure</u>

2.1 Filtering procedure

2.2 Closure for the Interphase Drag Force

2.3 Deep neural Network-Based Drag Corr…

<u>3. Dataset Creation and Marker Selection</u>

3.1 Marker Analysis and Preparation

<u>4. Results</u>

4.1 DNN models from Fully Periodic…

4.2 Fully Periodic 3D Domain

Muotoilu

<u>1 Background</u>

1.1 Solution-focused approach

1.2 Dual processing theory

1.3 Site analysis

<u>2 Aims</u>

<u>3 Method</u>

3.1 Participants

3.2 Interviewing technique

3.3 Data collection

3.4 Data-analysis

<u>4. The influence of type 1 on site analysis</u>

4.1 Narratives influencing the feeling of…

4.2 Substitution to reach information-satis…

<u>5 Motivational factors affecting individuals’…</u>

Keskivaiheen jäsennys
jäsennys strategiana

Lineaarinen	**Temaattinen**
Tutkimusvaihe 1	Menetelmä 1
Tutkimusvaihe 2	Menetelmä 2
…	…
Vaiheen 1 tulokset	Menetelmän 1 tulokset tai Teema 1
Vaiheen 2 tulokset	Menetelmän 2 tulokset tai Teema 2
…	…

Keskivaiheen jäsennys (tekstitaso)

- Niin lineaarinen kuin temaattinen strategia (painotus) edellyttävät tekstiltä *sidosteisuutta*
- Tekstin jäsennyksestä riippumatta sidosteisuuden lähteet ovat samanlaiset: sisällöt, terminologia, taakse- ja eteenpäin viittaavat ilmaukset, metateksti
- Lineaarisessa strategiassa korostuvat viittaukset tekstin (välittömästi) edeltävään ja seuraavaan tekstin osaan ja sisällöllinen + terminologinen sidosteisuus
- Temaattisessa strategiassa korostuvat tekstinosan yhteydet yläteemaan (yhdistävä nimittäjä) → yleinen käsittely pääluvun alussa (ja lopussa)

Luvun sisäinen rakenne:
Esitysjärjestys ja spesifisyys

Aalto-yliopisto
Aalto-universitetet
Aalto University

Paluu johdantoon: esitysjärjestys

Creating a Research Space

1. kappale: tausta (ilmiö yleisesti)

Hattivattien kanta on vuonna 1993 voimaan astuneen pyydystyskiellon myötä vakiintunut noin…

2. kappale: motivaatio (ratkaistava ongelma tai tutkimusaukko)

Hattivattien leviäminen tiiviin asututuksen alueille on johtanut hattivatteihin liittyvien liikenneonnettomuuksien…

3. kappale: aihe (ratkaisu ongelmaan tai tutkimusaukkoon)

Tässä tutkimuksessa kehitettiin yksinkertainen ja kustannustehokas menetelmä hattivattien houkuttelemiseksi…

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Sankaran Sundaresan[2]
Mohammadsadegh Salehi[1]
Stefan Radl[1]

Machine Learning-Based Filtered Drag Model for Cohesive Gas-Particle Flows

The accuracy of filtered two-fluid model simulations critically depends on constitutive models for corrections that account for the effects of inhomogeneous structures at the sub-grid level. The complexity of accounting these structures increases with cohesion. In the present study, a dataset from filtered Euler-Lagrange simulations with systematic variations of the cohesion level and the filter length was created to investigate the development of a machine learning-based drag correc-

The present contribution aims at developing a neural network-based drag correction function for […]

Supporting Information available online

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1 Introduction

Fine particles are widely used in various industrial sectors as they feature high specific surface area, which increases the rate of heat and mass transfer [1]. In the petrochemical industry, small catalyst particles are used in the fluid catalytic cracking process [2]. In the pharmaceutical industry, active pharmaceutical ingredients (APIs) are typically delivered as fine particles to improve the dissolution and release rate in the body [3]. In the food industry, fine powders are desirable due to their high specific surface area [4]. Unfortunately, these fine particles exhibit cohesive forces which critically impact powder flowability and fluidizability.

Powders featuring cohesive interactions can be categorized from mildly cohesive to highly cohesive. The level of cohesion can be quantified based on a Bond number, which describes the ratio of cohesion forces to the gravitational force. The cohesion can be due to the van der Waals forces or the presence of liquid bridges between the particles in the gas-solid systems. With the latter, one must consider viscous and surface tension forces, quantified via Bond and capillary numbers [5–7].

As cohesion originates from particle level interactions, its experimental quantification is challenging. However, detailed numerical simulation can help in analyzing the contribution of different forces to the strength of granules and powder flowability. Typically, two different approaches can be used in this regard: (i) an Euler-Euler simulation approach based on the two-fluid model (TFM) [8], or (ii) an Euler-Lagrange approach where the local-average equation for the fluid phase is simulated using computational fluid dynamics and the particle motion is followed via the discrete element method (CFD-DEM) [9]. Strictly speaking, both approaches need high grid resolution, which could render the simulations prohibitively expensive. To address this issue, filtered modeling approaches have been developed to permit accurate simulations of industrial-scale systems using coarse grid resolutions [10, 11].

The accuracy of the filtered two-fluid model (fTFM) approach depends critically on constitutive models for corrections that account for the effects of inhomogeneous structures at the sub-grid level [12]. The complexity of accounting for inhomogeneous structures increases for cohesive gas-particle flows [13].

In the literature, the drag force correction was identified as the most important feature in fTFMs [14, 15]. Several different approaches to constitute models for drag correction have been pursued in the literature [16]: (i) corrections based on the filter size and the resolved variables [12, 17–21], (ii) functional models that additionally use sub-filter level variables like the scalar variance of solid volume fraction [14, 21, 22], or (iii) the corrections based on a drift velocity (or flux) [15, 22–28] which recognizes that the filtered gas velocity and the (average) gas velocity seen by the particles are not the same. Here, the focus lies on the drift velocity-based approach.

Machine Learning (ML) techniques have recently been applied to develop drag force corrections: Jiang et al. [24, 25] formulated an artificial neural network (ANN) model to

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predict the drift velocity. Lu et al. [29] predicted the drag correction function directly based on an ANN. Zhu et al. [30] investigated the usage of an ANN (or an XGBoost) [31] regressor to predict the drag correction function. Zhang et al. [32] utilized a convolutional neural network (CNN) to model the drag correction function in a comparable system. These ML-based studies demonstrated improved drag correction modeling for non-cohesive systems, but none of them considered cohesive gas-particle flows or the possibility of anisotropy, i.e., a directional dependency of the drag correction.

Ozel et al. [22] investigated drag correction in cohesive systems, where the cohesion resulted from van der Waals-type

[…] uer [33] showed that an advanced stress modeling, among other improvements, positively impacts drag modeling. Zhu et al. [30] incorporated a particle phase Reynolds stress-like marker in their drag correction model. Also, Zhang et al. [32] suggested to use such a particle phase Reynolds stress-like marker in a drag correction model.

The present contribution aims at developing a neural network-based drag correction function for filtered simulations of cohesive gas-particle systems, where the cohesion comes from liquid bridges between particles. This is motivated by the fact that wet gas-particle systems are widely used in the chemical and pharmaceutical industry, e.g., for coating or granulation. We will compare our findings for drag corrections for dry gas-particle systems and cohesive systems where the cohesion is due to van der Waals interaction. Our model accounts for the anisotropy of drag correction.

To achieve these goals, highly resolved CFD-DEM-based simulations of wet gas-particle fluidization were performed to generate computational data on the mesoscale structures. Then, these results were systematically filtered, using different filter sizes, to obtain datasets on flow quantities that are relevant for fTFM development. The closure relations for the fTFM of the wet gas-particle systems were then constructed.

2 Model Description and Filtering Procedure

Highly resolved CFD-DEM simulations for a range of conditions are performed. The CFD part is realized within the framework of OpenFOAM® [34], and the DEM part is solved using LIGGGHTS® [35]. The coupling between these two tools is performed with CFDEM® [35]. The detailed CFD-DEM equations can be found in the Supporting Information.

2.1 Filtering Procedure

Filtering operations are performed via the tool CPPPO [36]. The filtered solid volume fraction is:

$$\bar{\phi}_s(\mathbf{x},t) = \int\int\int \phi_s(\mathbf{r},t)\, G(\mathbf{r}-\mathbf{x})\, d\mathbf{r} \qquad (1)$$

where $\mathbf{x}$ is the spatial position (any position in the grid), $\mathbf{r}$ is an independent spatial coordinate. The box filter (top-hat) kernel $G(\mathbf{r}-\mathbf{x})$ is normalized so that $\int\int\int G(\mathbf{r}-\mathbf{x})d\mathbf{r} = 1$ and is defined by the fluid filter size Δ_f after:

$$\ldots \begin{cases} \frac{1}{\Delta_f^3}, & \text{if } |\mathbf{r}-\mathbf{x}| \le \frac{\Delta_f}{2} \\ 0, & \text{otherwise} \end{cases} \qquad (2)$$

[…]ed gas and solid velocities, as well as the filtered gas […] given by:

$$\ldots \frac{1}{(1-\bar{\phi}_s)} \int\int\int G(\mathbf{r}-\mathbf{x})(1-\phi_s(\mathbf{r},t))\, \mathbf{u}_g(\mathbf{r},t)\, d\mathbf{r} \qquad (3)$$

$$\tilde{\mathbf{u}}_s(\mathbf{x},t) = \frac{1}{\bar{\phi}_s} \int\int\int G(\mathbf{r}-\mathbf{x})\, \phi_s(\mathbf{r},t)\, \mathbf{u}_s(\mathbf{r},t)\, d\mathbf{r} \qquad (4)$$

$$\bar{p}(\mathbf{x},t) = \int\int\int G(\mathbf{r}-\mathbf{x})\, p(\mathbf{r},t)\, d\mathbf{r} \qquad (5)$$

Eulerian solid velocity $\mathbf{u}_s$ is the Lagrangian particle velocity mapped onto the Eulerian grid (for details see Supporting Information). For the filtered mass and momentum conservation equations also see the Supporting Information.

2.2 Closure for the Interphase Drag Force

The filtered Eulerian drag force

$$\Phi_d = \overline{\beta^{Eul}(\mathbf{u}_g-\mathbf{u}_s)} = \bar{\beta}^{Eul}(\tilde{\mathbf{u}}_g-\tilde{\mathbf{u}}_s) \qquad (6)$$

needs to be closed in filtered simulations. Here, β^{Eul} is the drag coefficient estimated using local particle volume fraction and the local velocities. The specific drag law used in this study is that due to Beetstra et al. [37]. Details about the drag law and drag coefficient calculation can be found in the Supporting Information. $\bar{\beta}^{Eul}$ is the filtered Eulerian drag coefficient that needs to be found. Following Ozel et al. [22], one can write:

$$\Phi_d = \bar{\beta}^{Eul}(\tilde{\mathbf{u}}_g-\tilde{\mathbf{u}}_s) \approx \Phi_{d,A} = \beta^{Micro}(\tilde{\mathbf{u}}_g-\tilde{\mathbf{u}}_s+\tilde{\mathbf{v}}_d) \qquad (7)$$

Here, β^{Micro} is the drag coefficient evaluated based on filtered quantities using the same drag law used to find β^{Eul}. The sub-grid drift velocity $\tilde{\mathbf{v}}_d$ is defined by:

$$\tilde{\mathbf{v}}_d = \frac{\overline{\phi_s \mathbf{u}_g}}{\bar{\phi}_s} - \tilde{\mathbf{u}}_g \qquad (8)$$

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Keywords: Cohesive gas-particle flow, Drag correction model, Filtered simulations, Machine learning

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Fine particles are widely used in various industrial sectors as

Unfortunately, these fine particles exhibit cohesive forces which

As cohesion […] experimental quantification is challenging. However, detailed numerical simulation can help […]

Euler-Euler simulation approach based on the two-fluid model (TFM)

The accuracy of […] (fTFM) depends […] models for corrections

drag force correction was identified as the most important feature in fTFMs

Machine Learning (ML) techniques have recently been applied to develop drag force corrections

1. tausta (ilmiö yleisesti)

Fine particles are widely used in various industrial sectors as

2. ongelma

Unfortunately, these fine particles exhibit cohesive forces which

3. lisäongelma, potentiaalinen ratkaisutyyppi

As cohesion […] experimental quantification is challenging. However, detailed numerical simulation can help […]

4. Konkreettinen ratkaisu

Euler-Euler simulation approach based on the two-fluid model (TFM)

5. Konkreettisen ratkaisun lähtöedellytys (tyyppi)

The accuracy of […] (fTFM) depends […] models for corrections

6. Tietty lähtöedellytys

drag force correction was identified as the most important feature in fTFMs

7. Lähtöedellytyksen ratkaisu

Machine Learning (ML) techniques have recently been applied to develop drag force corrections

Mitä jos…

1) **Tausta ml. sovellukset** *Fine particles are … In industry …*
2) **Ongelmat kimppuna, ml. sovellukset** *Cohesion… numerical modelling expensive ... fTMS … none of them considered…*
3) **Ratkaisu** *The present contribution…*
4) **Tutkimuksesta/sovelluksesta tarkemmin** […]
5) **Ongelmista tarkemmin** […]
6) **Ratkaisusta tarkemmin** […]

Kerronnan strategiat

Ketju

- Teksti seuraa ilmiöiden välisiä yhteyksiä
- Lineaarinen/kronologinen
- Sama (korkea) spesifisyyden aste
- Metatekstiä vähän / myöhään

Kehys

- Teksti lähestyy ilmiön ydintä asteittain
- Syklinen
- Vaihteleva spesifisyyden aste
- Metatekstiä paljon / aikaisin

Aloituksesta

Osmolska & Lewis (2023)

Architects' use of intuition in site analysis: Information gathering in solution development

Design Studies

4 *The influence of type 1 on site analysis*

The findings below explore themes related to how site analysis is conducted in the real world, and to the influence of Type 1 on the development of solutions and information-gathering judgements.

4.1 *Narratives influencing the feeling of solution-satisfaction*

Information for site analysis is often gathered in stages (some information might come sooner and some later) [A2, 4, 6, 7, 8, 9, 10, 12, 14, 15, 18, 21].

- **Metateksti.** Miten tulokset ("findings") on järjestetty =
- Teemoittain ja suhteessa esitettyyn ratkaisustrategiaan (Type 1)

Tausendschön ym. (2023)
Machine Learning-Based Filtered Drag Model for Cohesive Gas-Particle Flows

Chem. Eng. Technol. 2023

- **Yleinen metodologinen huomio**
- **Aikaisempia tuloksia**
- **Yleinen luonnehdinta tuloksista**

4 Results

The overall accuracy of a model is typically assessed by comparing the predicted and target values of suitable output variables. Lu et al. [29] compared predicted and target values of H_d but did not show the analogous comparison of the filtered drag force. Jiang et al. [25] found a Pearson correlation coefficient of 0.99 for the filtered drag force model. Zhu et al. [30] obtained a Pearson correlation coefficient of ~ 0.98 for H_d. Zhang et al. [32] found that their Pearson correlation coefficient values ranged between ~ 0.7 and ~ 0.9, while R^2 values were between ~ 0.5 and ~ 0.8, depending on the filter size.

The filtering procedure used to create the datasets was validated against literature data (see part E in the Supporting Information for details). Further, the adequacy of Eq. (7) was