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Version 1

An Open-source Aerosol Dynamics and Computational Fluid Dynamics Model

aerosolGDEFoam User Guide

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Source

- Woo et al. “Open-source Aerosol Dynamics and Computational Fluid Dynamics 2 Model: Nodal Method for Nucleation, Coagulation, and Surface growth”, Journal, year, page. doi

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Contents

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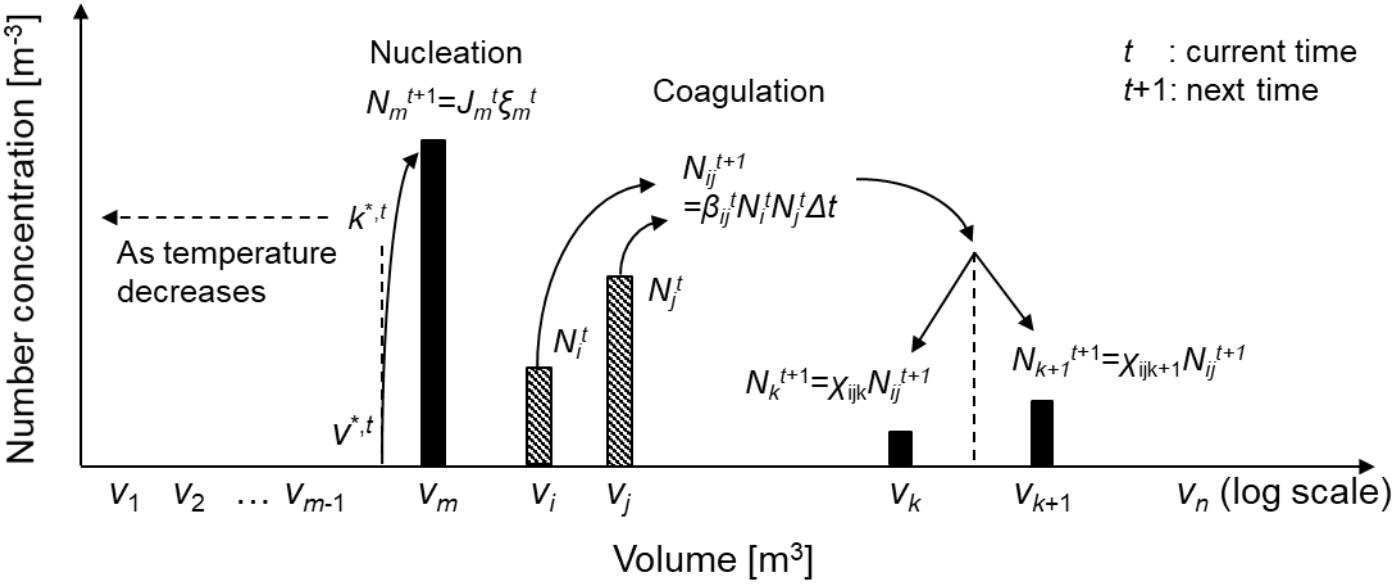
1. Introduction

- Implementation of nodal method for time dependent general dynamic equation including nucleation, surface growth, and coagulation mechanisms



Schematics of nucleation and coagulation algorithms in nodal method

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1. Introduction

- Governing equations

Particles

$$\frac{\mathrm{d}N_k}{\mathrm{d}t} = \underbrace{J_k \xi_k}_{\text{nucleation}} + \underbrace{\frac{1}{2}\sum_{\substack{i=2\\ j=2}} \chi_{ijk}\beta_{i,j}N_i N_j - N_k \sum_{i=2}\beta_{i,k}N_i}_{\text{coagulation}}$$

$$+ \underbrace{\begin{cases} \dfrac{v_1}{v_k - v_{k-1}}\beta_{1,k-1}(N_1 - N_{\mathrm{sat},1,k-1})N_{k-1} & \text{if } N_1 > N_{\mathrm{sat},1,k-1} \\ -\dfrac{v_1}{v_{k+1} - v_k}\beta_{1,k+1}(N_1 - N_{\mathrm{sat},1,k+1})N_{k+1} & \text{if } N_1 < N_{\mathrm{sat},1,k+1} \\ -\dfrac{v_1}{v_{k+1} - v_k}\beta_{1,k}(N_1 - N_{\mathrm{sat},1,k})N_k & \text{if } N_1 > N_{\mathrm{sat},1,k} \\ \dfrac{v_1}{v_k - v_{k-1}}\beta_{1,k}(N_1 - N_{\mathrm{sat},1,k})N_k & \text{if } N_1 < N_{\mathrm{sat},1,k} \end{cases}}_{\text{surface growth}}$$

Monomer

$$\frac{\mathrm{d}N_1}{\mathrm{d}t} = J_1\xi_1 + \begin{cases} -\beta_{1,k-1}(N_1 - N_{\mathrm{sat},1,k-1})N_{k-1} & \text{if } N_1 > N_{\mathrm{sat},1,k-1} \\ -\beta_{1,k+1}(N_1 - N_{\mathrm{sat},1,k+1})N_{k+1} & \text{if } N_1 < N_{\mathrm{sat},1,k+1} \\ -\beta_{1,k}(N_1 - N_{\mathrm{sat},1,k})N_k & \text{if } N_1 > N_{\mathrm{sat},1,k} \\ -\beta_{1,k}(N_1 - N_{\mathrm{sat},1,k})N_k & \text{if } N_1 < N_{\mathrm{sat},1,k} \end{cases}$$

Nucleation rate

$$J_k = N_{\mathrm{sat}}^2 S v_1 \left(\frac{2\sigma}{\pi m_1}\right)^{0.5} \exp\left(\theta - \frac{4\theta^3}{27\log^2 S}\right)$$

Size operator

$$\xi_k = \begin{cases} \dfrac{v^*}{v_k}; & \text{if } v_{k-1} \le v^* \le v_k, \\ \dfrac{v^*}{v_2}; & \text{if } v^* \le v_1, \\ 0; & \text{otherwise} \end{cases}$$

Collision frequency

- Free molecular regime (Kn>10)

$$\beta_{ij} = \left(\frac{3}{4\pi}\right)^{1/6}\left(\frac{6k_{\mathrm{B}}T}{\rho_{\mathrm{p}}}\right)^{1/2}\left(\frac{1}{v_i} + \frac{1}{v_j}\right)^{1/2}\left(v_i^{1/3} + v_j^{1/3}\right)^2$$

- Continuum regime (Kn <<1)

$$\beta_{ij} = 2\pi(D_i + D_j)(d_i + d_j) \times \left[\frac{d_i + d_j}{d_i + d_j + 2(g_i^2 + g_j^2)^{1/2}} + \frac{8(D_i + D_j)}{\left(\bar{c}_i^2 + \bar{c}_j^2\right)^{1/2}(d_i + d_j)}\right]^{-1}$$

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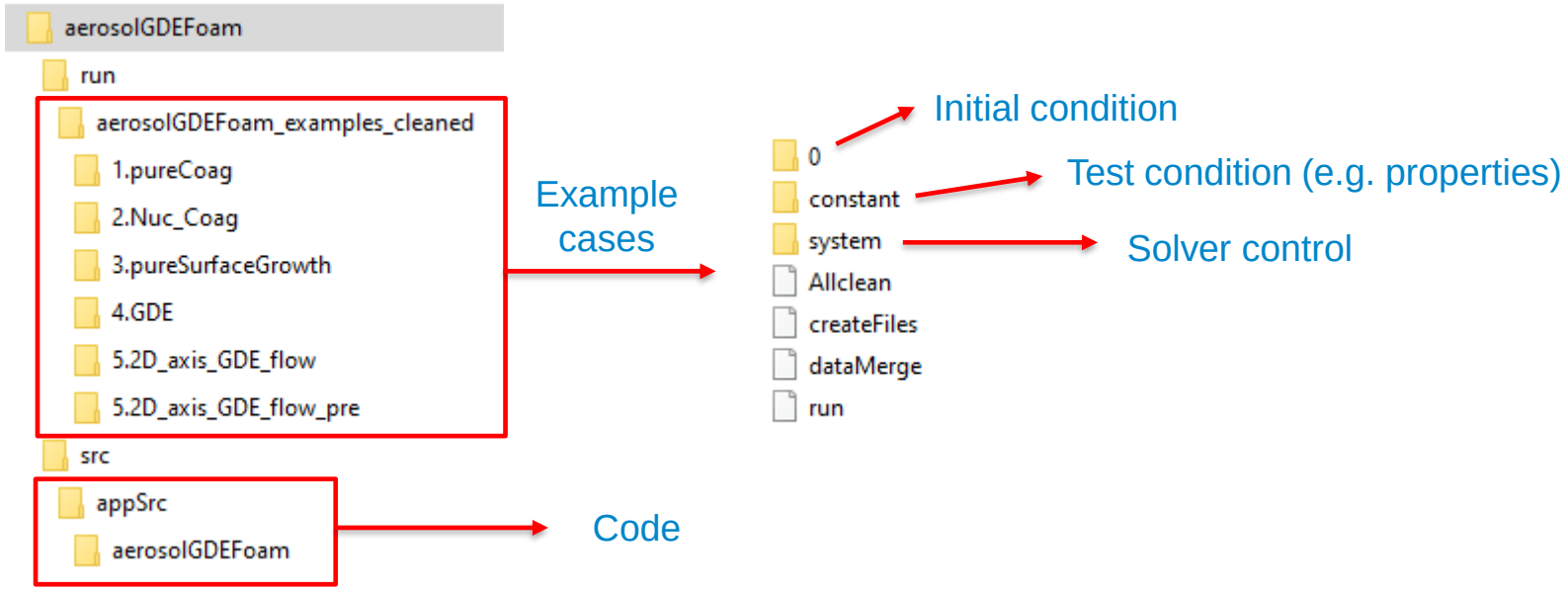
2. Code structure

- Developed on OpenFOAM 6 from The OpenFOAM Foundation
  - For download and install, visit https://openfoam.org/version/6/

- File structure



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2. Code structure

- constant/transportProperties

```
// * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * * //
coolrate    coolrate [0 0 -1 1 0 0 0] 1000;

mwParticle mwParticle [1 0 0 0 -1 0 0] 0.026981539; // Molecular weight(kg/mol)
rhoParticle  rhoParticle [1 -3 0 0 0 0 0] 2700; // Particle density (kg/m3)
surTens_A  surTens_A [1 0 -2 0 0 0 0] 948; // Surface tension coefficient
surTens_B  surTens_B [1 0 -2 -1 0 0 0] 0.202; // Surface tension coefficient
satVap_A  satVap_A [0 0 0 0 0 0 0] 13.07; // Saturation vapor pressure coefficient
satVap_B  satVap_B [0 0 0 1 0 0 0] 36373; // Saturation vapor pressure coefficient
```

Parameters for nucleation rate by self-consistent correction (SCC) model*, Eq. (5) in the paper

$$J_k = n_{\text{sat}}^2 S v_1 \left(\frac{2\sigma}{\pi m_1}\right)^{0.5} \exp\left(\theta - \frac{4\theta^3}{27\log^2 S}\right)$$

$p_{\text{sat}} = p\exp(13.07 - 36373/T)$: Saturation pressure

$\sigma = (948 - 0.202T)/1000$: Surface tension

*Reference: Girshick, S. L., and Chiu, Chia Pin. (1990). Kinetic Nucleation Theory: A New Expression for the Rate of Homogeneous Nucleation from an Ideal Supersaturated Vapor, J. Chem. Phys. 93:1273–1277.

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2. Code structure

- constant/transportProperties (cont.)

```
nodes nodes [0 0 0 0 0 0 0] 41; // number of nodes
```

Node spacing according to the Eq. (1) and (2) in the paper

$$v_k = v_1 q^k \quad \text{and} \quad q = 10^{\frac{12}{k_{max}-2}}$$

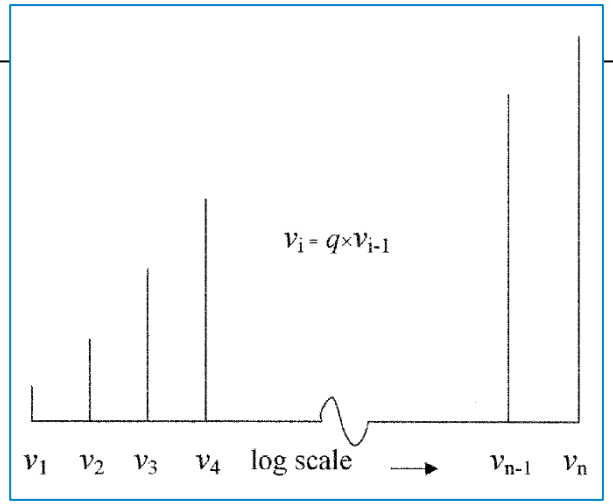

Figure: Illustration of node spacing on a logarithmic volume space where q is the geometric spacing factor*

```
nucleation    true;
coagulation   true;
growth        false;
advection     false;
// ********************************************************************************* //
```

Choose the models of interest

*Ref.: A simple numerical algorithm and software for solution of nucleation, surface growth, and coagulation problems, Prakash et al., Aerosol Science Technology, 37:892-898, 2003.

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2. Code structure

- system/controlDict

```
                                    ⋮
startFrom       startTime;//latestTime   Start from initial condition or restart at latest time
startTime       0;
stopAt          endTime;
endTime         1.3745;                  Time at which the simulation ends
deltaT          0.0001;                  Time step
writeControl    timestep;//adjustableRunTime   Write based on time step or time
writeInterval   2749;//0.2749            Write interval based on time step or time
                                    ⋮
```

- For more details on the usage of controlDict in OpenFOAM 6
  - https://cfd.direct/openfoam/user-guide/v6-controldict/

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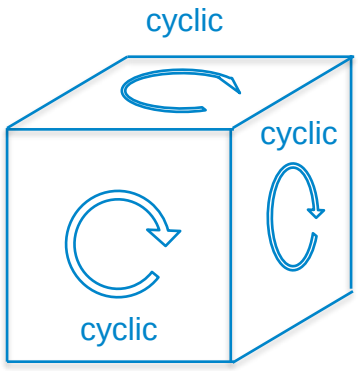
3. Verification cases: general dynamic equation (GDE) without flow

- Test problem: time evolution of monomer and particles
  - Zero dimensional problem dependent only on time
  - For pure coagulation (1.pureCoag)
    - Self-preserving distribution from monodisperse particles at the smallest node
  - For the other examples (2.NucCoag, 3.pureSurfaceGrowth, 4.GDE)
    - Aluminum particle formation and growth from a vapor at 1773K as it is passed into a condenser with a cooling rate of 1000K/s*.
- Computational domain
  - Cubic domain with cyclic boundary conditions for each pair of opposite faces



- 1×1×1 unit cell for uniform field (no spatial difference)
- Enable 0D simulation by OpenFOAM based on 3D solver

*Ref.: Panda, S. and S.E. Pratsinis, *Modeling the synthesis of aluminum particles by evaporation-3 condensation in an aerosol flow reactor.* Nanostructured Materials, 1995. **5**(7): p. 755-767

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3. Verification cases: general steps to setup the test case

- Pre-step 1: Generate mesh
  - Go to run folder (e.g. ./1.pureCoag/40) and ./system/blockMeshDict

```
                ⋮

vertices
(
    (0 0 0)      //0
    (1 0 0)      //1
    (1 1 0)      //2
    (0 1 0)      //3
    (0 0 1)      //4
    (1 0 1)      //5
    (1 1 1)      //6
    (0 1 1)      //7
);
blocks
(
    hex (0 1 2 3 4 5 6 7) block1 (1 1 1)
simpleGrading (1 1 1)
);
edges
(
);
```

Domain geometry

```
Boundary
(
    front
    {
        type cyclic;
        neighbourPatch back;
        faces
        (
            (4 5 6 7)
        );
                    ⋮
```

Boundary conditions of front (identical for other boundaries)

Mesh cells and grading

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3. Verification cases: general steps to setup the test case

- Pre-step 2: Compile
  - Go to source folder cd src/appSrc/aerosolGDEFoam
  - ./wmake

- Pre-step 3: Data creation before running
  - Go back to run folder and ./createFiles

    Create a number of files depending on the number of nodes defined in constant/tranportProperties

    Initial condition should be specified after file creation

- Post-step: data merging for verification cases
  - In run folder ./dataMerge

    Take the lines for number concentrations at each node and merge

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3.1 Pure coagulation

- Step 1: test condition
  - Go to ./constant/transportProperties
  - Set the number of node, coolrate and models

```
coolrate    coolrate [0 0 -1 1 0 0 0] 0;

mwParticle  mwParticle [1 0 0 0 -1 0 0] 0.026981539; // Molecular weight(kg/mol)
rhoParticle  rhoParticle [1 -3 0 0 0 0 0] 2700; // Particle density (kg/m3)
surTens_A  surTens_A [1 0 -2 0 0 0 0] 948; // Surface tension coefficient
surTens_B  surTens_B [1 0 -2 -1 0 0 0] 0.202; // Surface tension coefficient
satVap_A  satVap_A [0 0 0 0 0 0 0] 13.07; // Saturation vapor pressure coefficient
satVap_B  satVap_B [0 0 0 1 0 0 0] 36373; // Saturation vapor pressure coefficient

nodes nodes [0 0 0 0 0 0 0] 41; // number of nodes

nucleation   false;
coagulation  true;
growth       false;
advection    false;
```

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3.1 Pure coagulation

- Step 2: Set initial condition
  - Run ./createFile
  - Go to ./0 and open nPartNode2

```
dimensions      [0 -3 0 0 0 0 0];
internalField   uniform 1e24;
boundaryField
{
    front
    {
        type
            cyclic;
    }
    back
    {
        type
            cyclic;
    }
```

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3.1 Pure coagulation

- Step 3: solver control
  - Go to ./system/controlDict
  - Setup time step and write interval

```
application     scalarTransportFoam;

startFrom       latestTime;

startTime       0;

stopAt          endTime;

endTime         1e-6;

deltaT          1e-11;

writeControl    adjustableRunTime;

writeInterval   1e-7;
```

- Step 4: Restart with increased time step depending on characteristic coagulation time

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3.1 Pure coagulation

- Summary of test conditions

Number of nodes	41, 71 and 101
Initial concentration	nPartNode2: 1e24
Coolrate	0
Time step	Depending on characteristic coagulation time*
Models	nucleation false; coagulation true; growth false; advection false;

*Note:
- Time step is initially given as 1e-11 and increased when restart
- Self-preserving distribution is eventually obtained with time step higher than the criteria but with significant mass defect (valid only for pure coagulation)

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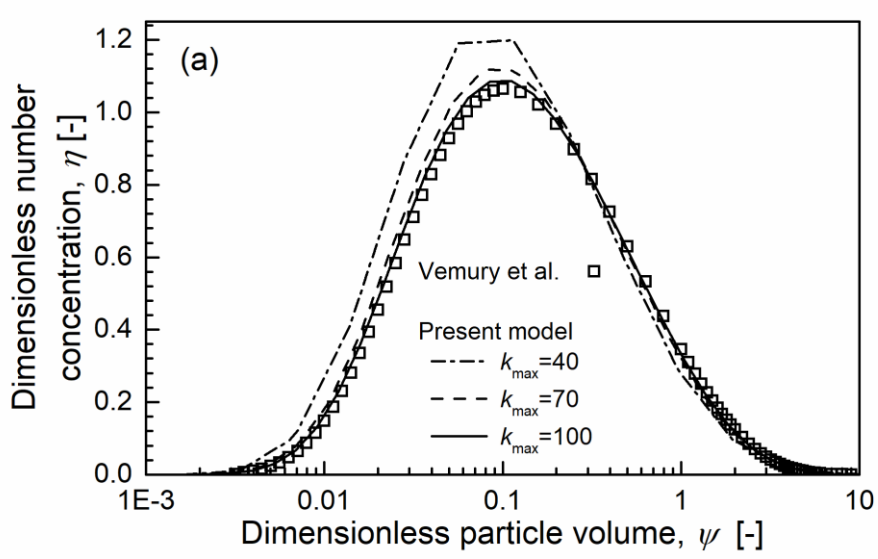
3.1 Pure coagulation

- Result



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3.2 Nucleation and coagulation

- Test conditions

Number of nodes	41
Initial concentration	nPartNode1: 2.4214e21
Coolrate	1000
Time step	1e-4
Models	nucleation true; coagulation true; growth false; advection false;

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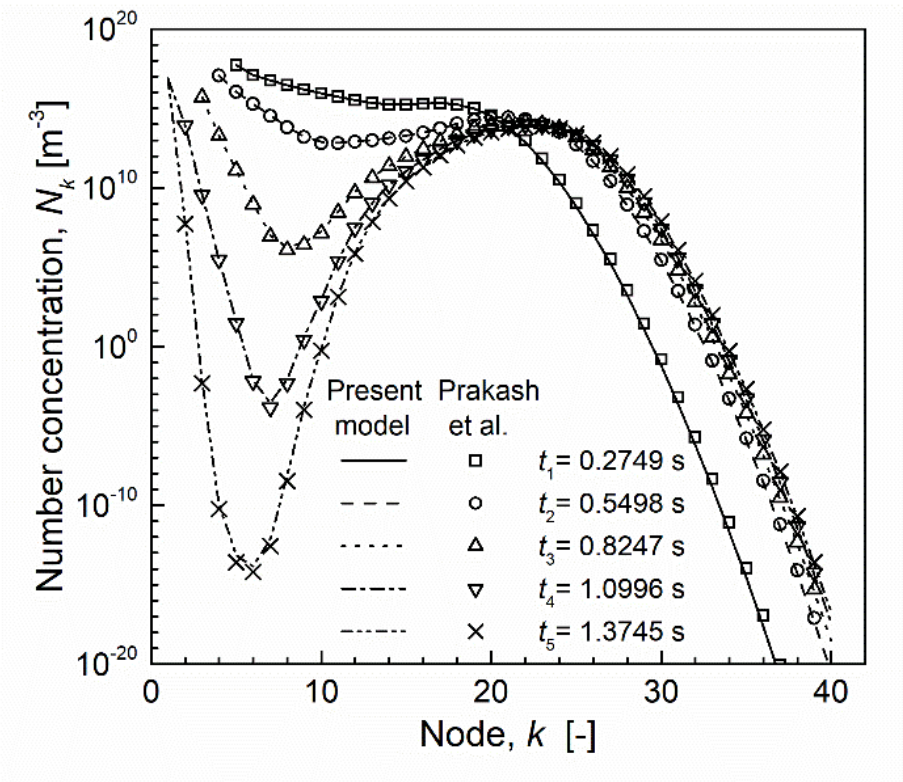
3.2 Nucleation and coagulation

- Result



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3.3 Pure surface growth

- Test conditions

Number of nodes	41
Initial concentration	nPartNode1: 2.4214e21 nPartNode25: 1e10
Coolrate	1000
Time step	1e-6
Models	nucleation false; coagulation false; growth true; advection false;

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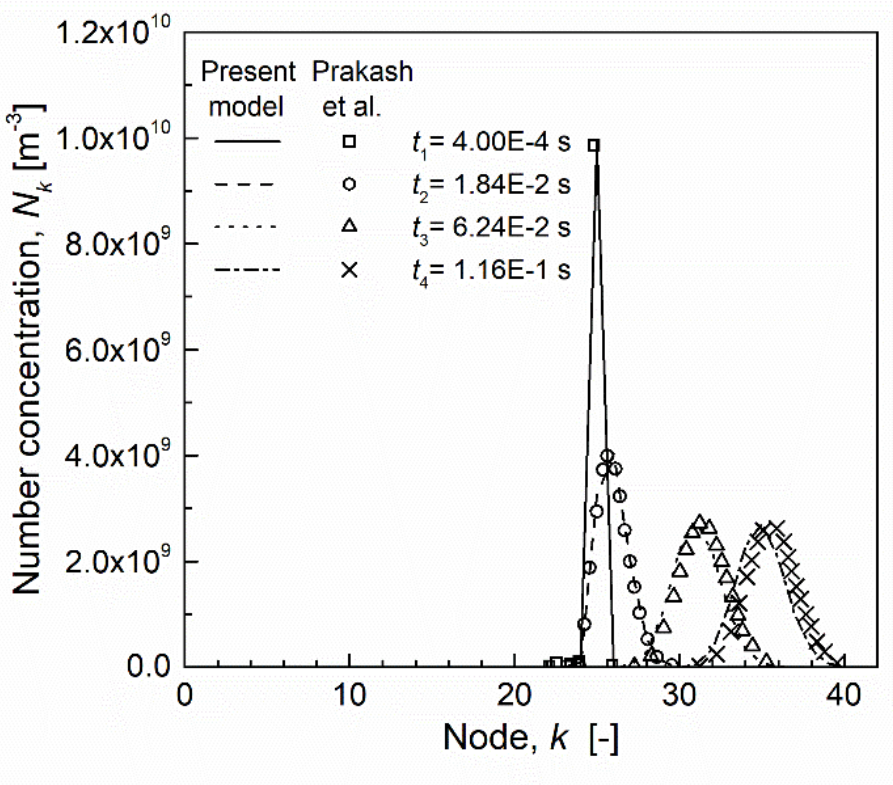
3.3 Pure surface growth

- Result



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3.4 GDE

- Test conditions

Number of nodes	41
Initial concentration	nPartNode1: 2.4214e21
Coolrate	1000
Time step	1e-5
Models	nucleation true; coagulation true; growth true; advection false;

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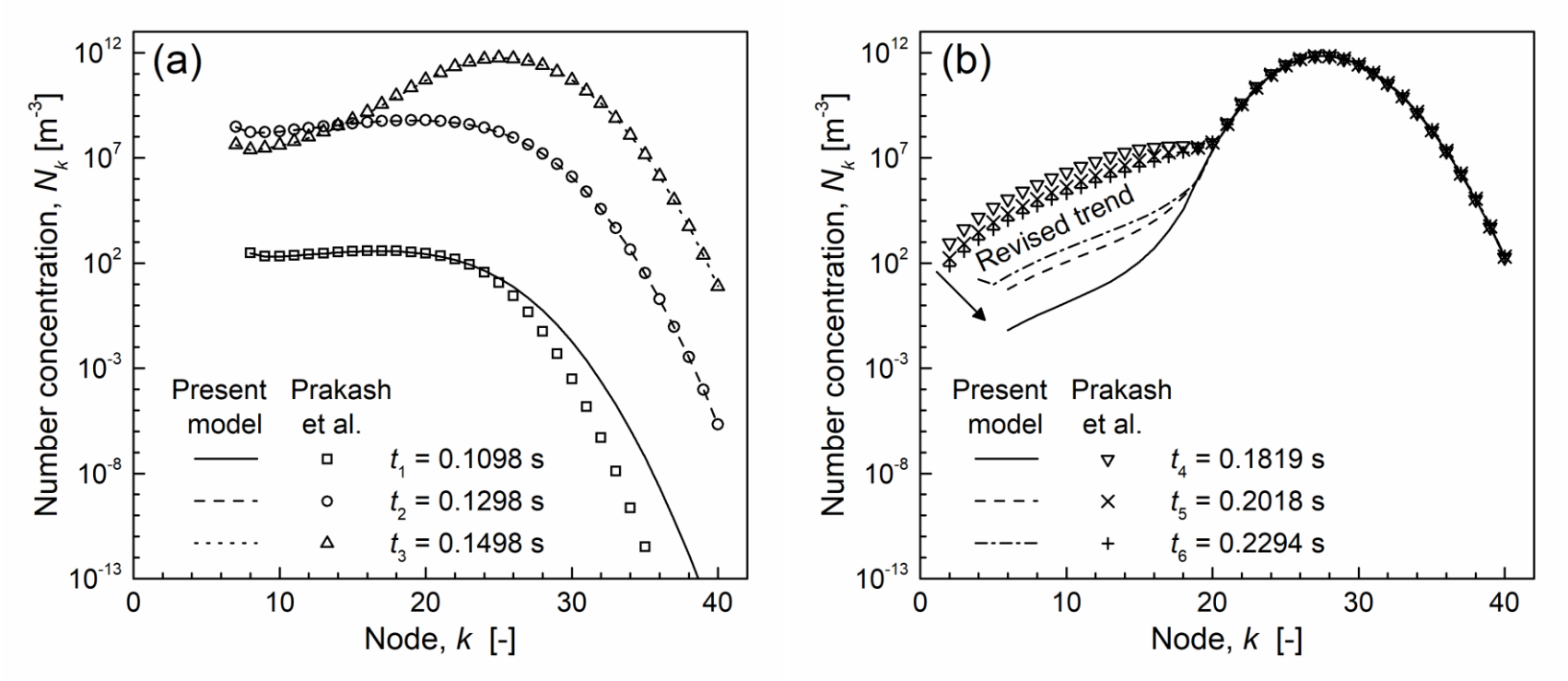
3.4 GDE

- Result



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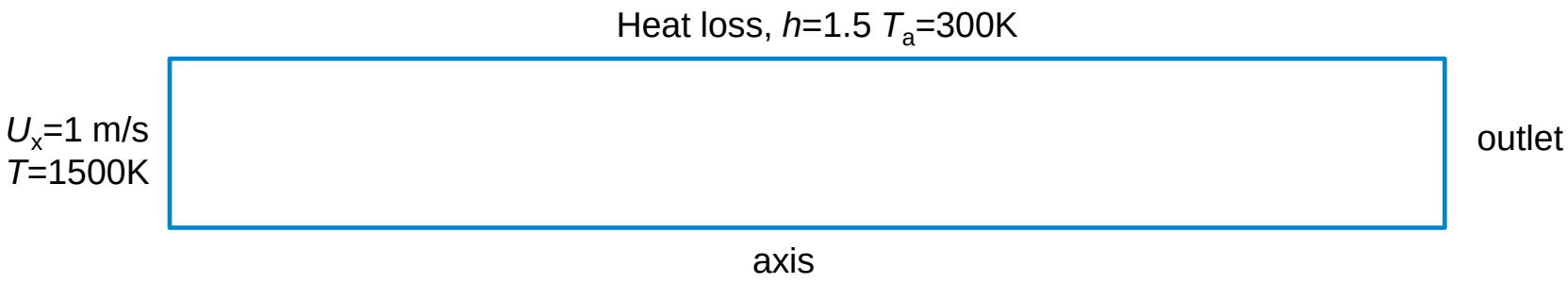
4. Example case with flow

- Pre-calculation
  - 2D axisymmetric computational domain and boundary conditions



  - Mesh
    - 200 ×20×1 2D axisymmetric mesh

```
blocks(    hex (0 3 4 1 0 3 5 2) block1 (200 20 1)     simpleGrading (5 0.1 1) );
```

  - Solver
    - rhoSimpleFoam

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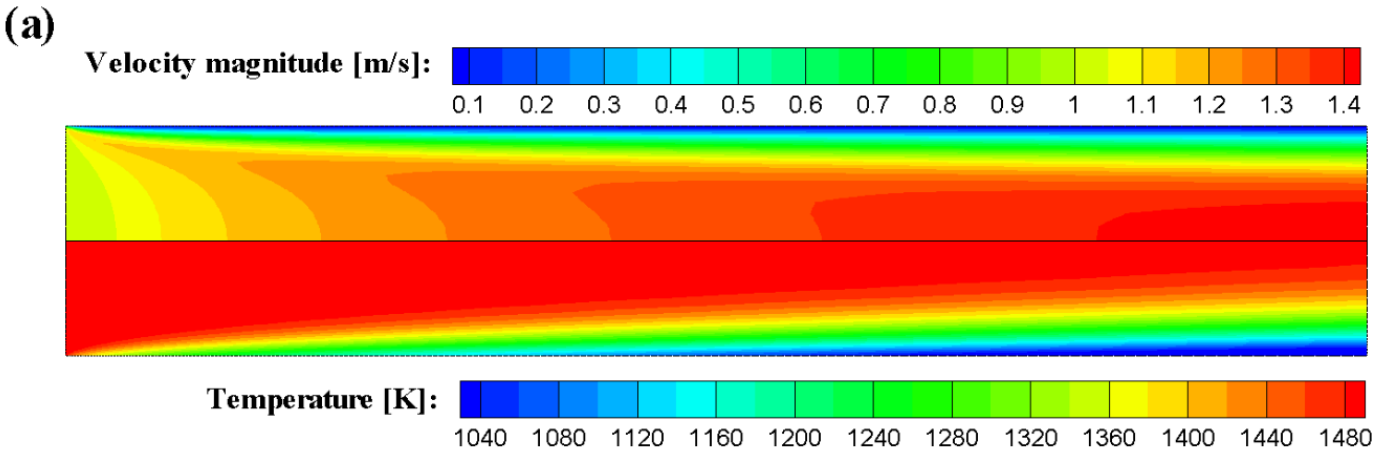
4. Example case with flow

- Results



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4. Example case with flow

- Copy
  - U,T,p from precalculation

- Test conditions

Number of nodes	41
Initial concentration	_nPart: 1e10 (before createFiles)
Coolrate	0
Time step	1e-5
Models	nucleation true; coagulation true; growth true; advection true;

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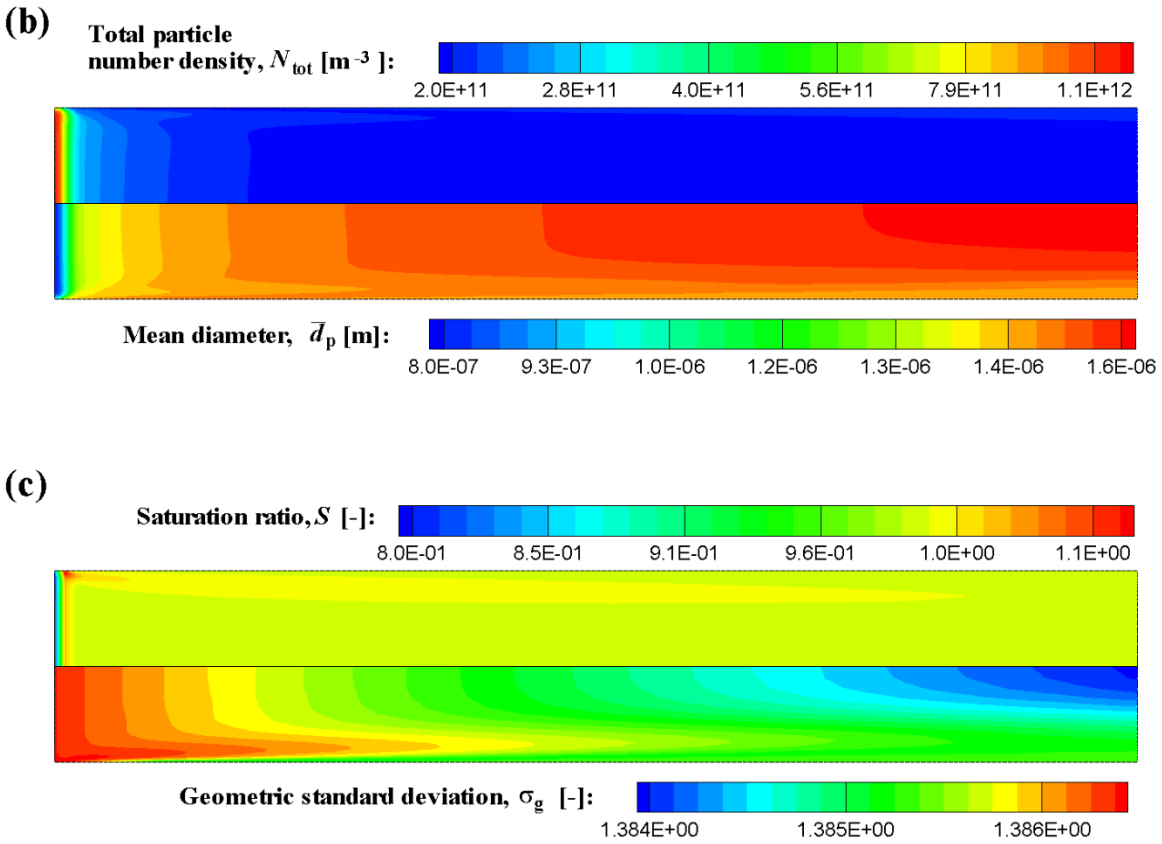
4. Example case with flow

- Results



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Thank you