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Numerical Simulation Examples by RFLOW

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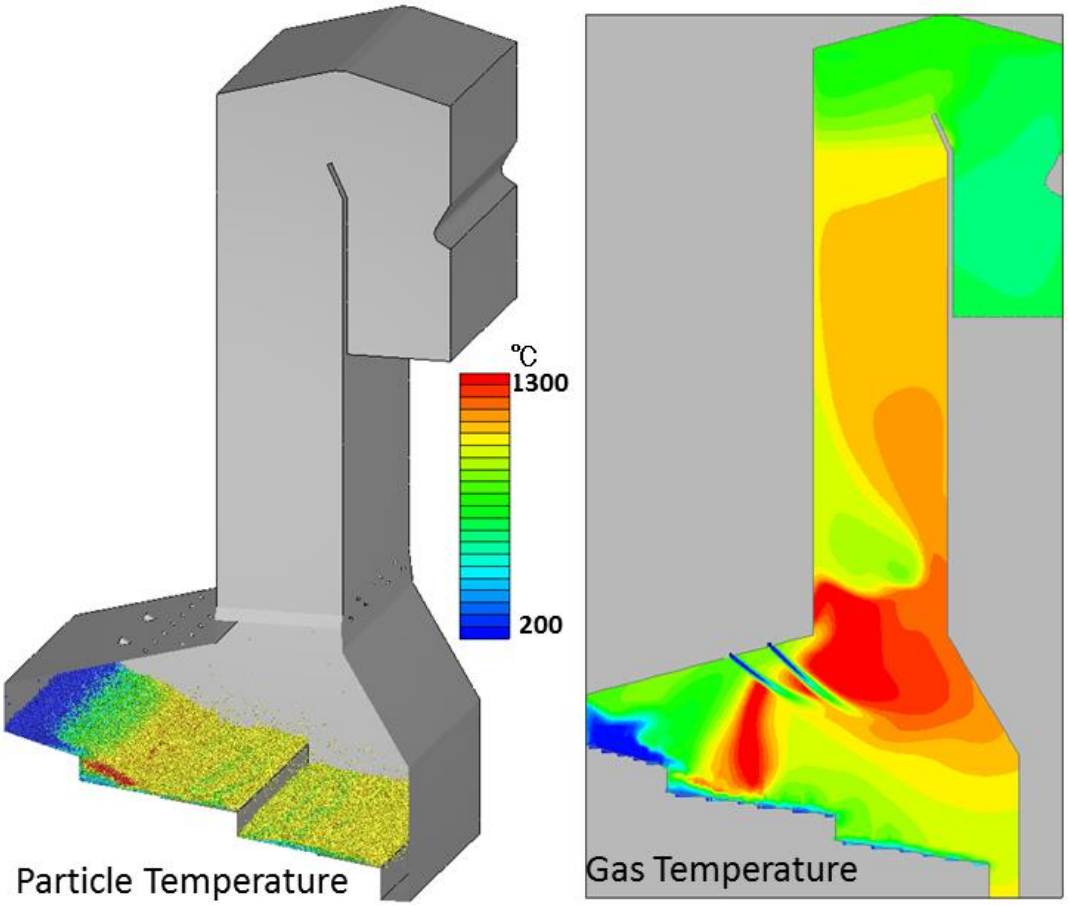
Combustion Simulation of Municipal Waste in Stoker Incinerator

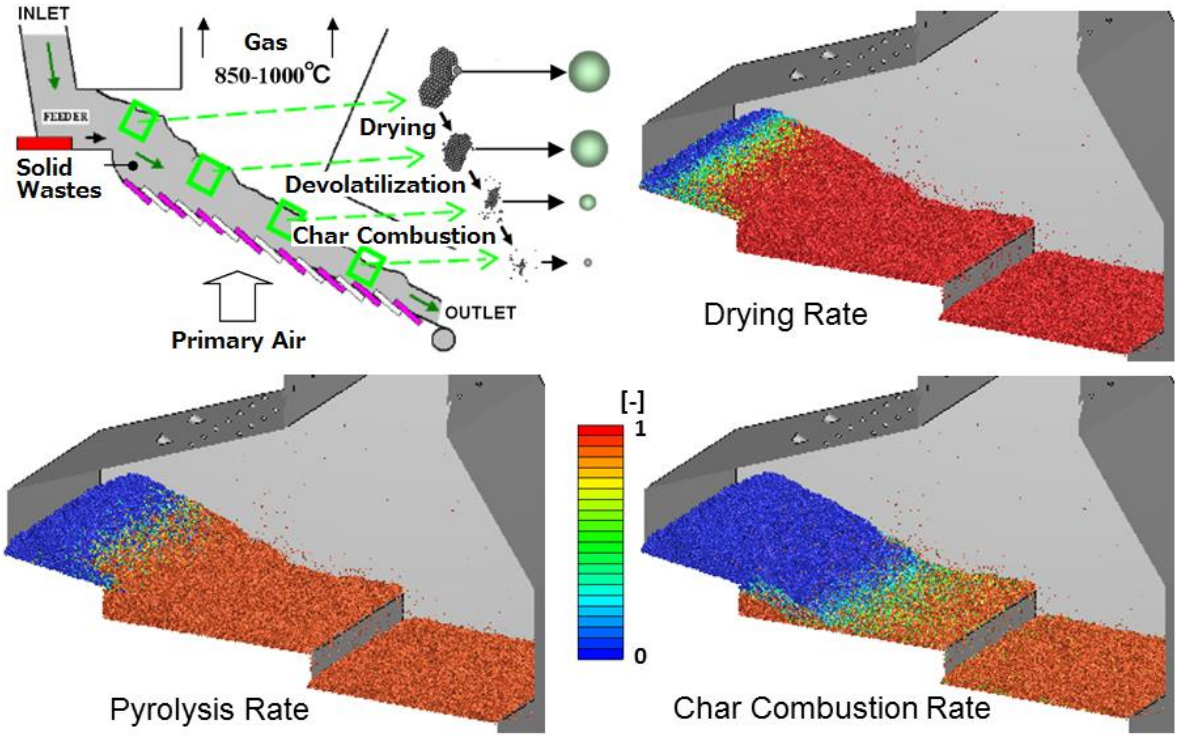
The municipal solid waste combustion process in a stoker-type incinerator with a capacity of 750 t/day, constructed several years ago in Guangdong Province, China, is numerically simulated. In the simulation, our originally developed "Representative Particle Model" [1, 2], which is a pioneer of the DEM (Discrete Element Method) based coarse-grained model, is used to simulate the behavior and combustion process of solid waste particles, coupled with the compressible flow of reactive gases and the radiation field. In addition, the combustion of solid waste particles is modeled in three stages: water evaporation, devolatilization (pyrolysis), and fixed carbon (char) combustion. Furthermore, each concentration component of reactive gases produced and extinguished during combustion process is also simulated such as Oxygen (O_2), water vapor (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4) and hydrogen (H_2).



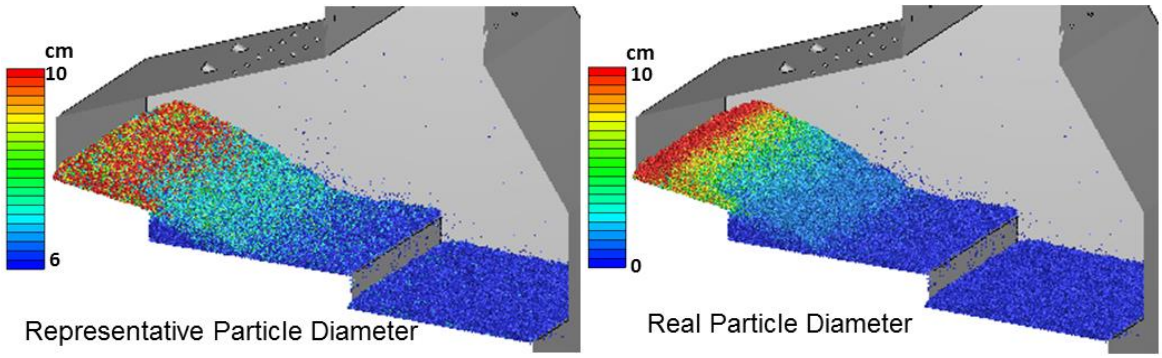
References

Takeda, H., Granular flow simulation by continuum model, J. Soc. Powder Technol., Japan. **40** 746-754 (2003)

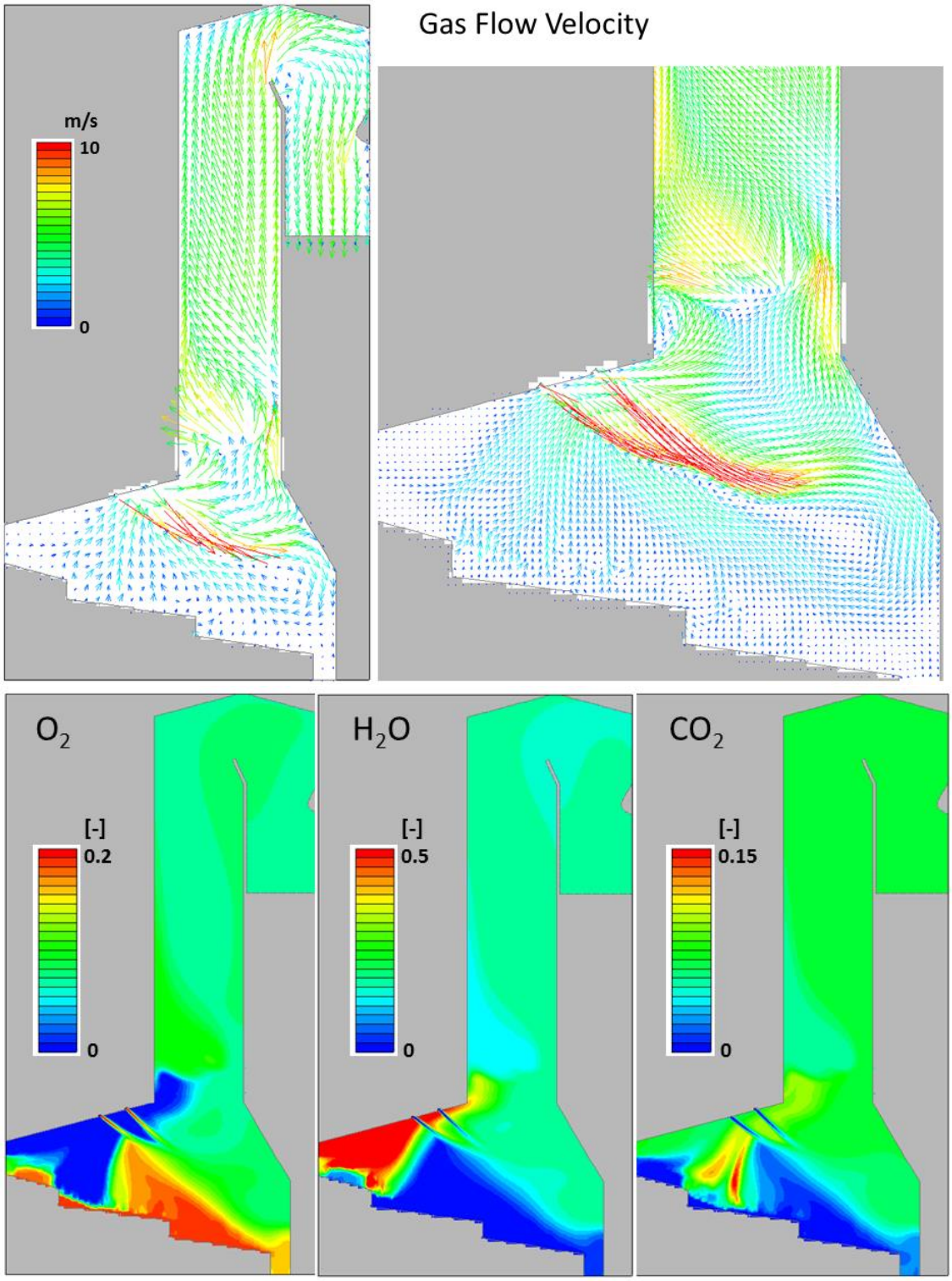
Takeda, H., Granular flow simulations in the industrial sector, J. Soc. Powder Technol., Japan. **50** 264-271 (2013)



The combustion process of solid waste particles is simulated in three stages: water evaporation, devolatilization (pyrolysis), and fixed carbon (char) combustion.



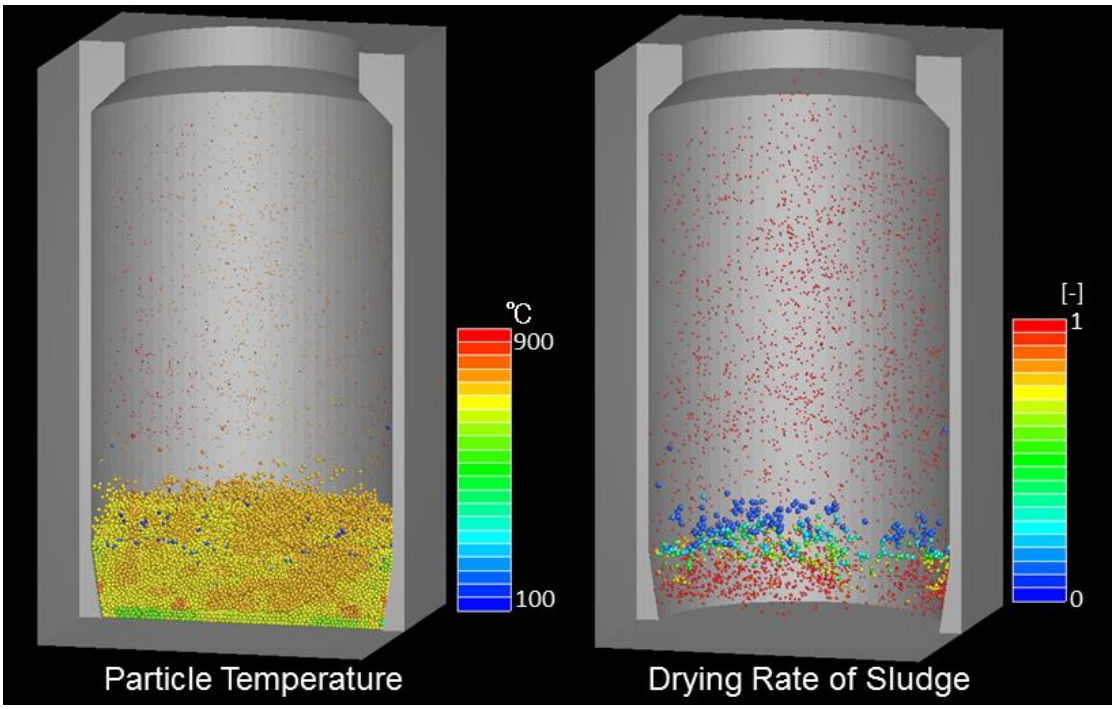
In the representative particle model, both the representative particle diameter (used to calculate the contact between particles) and the real particle diameter (the particle diameter of actual solid waste particles) change as the combustion progresses. The representative particle diameter is determined to reflect the particle volume decrease (mass decrease and density change). On the other hand, the actual particle diameter change is given as a simulation condition considering not only the change of the representative particle diameter but also the cracking of solid waste particles. In practice, the actual particle diameter distribution is specified at the time of waste particle generation and at the time of completion of combustion (when the particles are reduced to ash), and the intermediate stage is calculated by interpolation. Considering the actual particle diameter distribution at the completion of combustion and specifying it from the order of microns to cm as a simulation condition, the ratio of main ash to fly ash can be controlled indirectly.

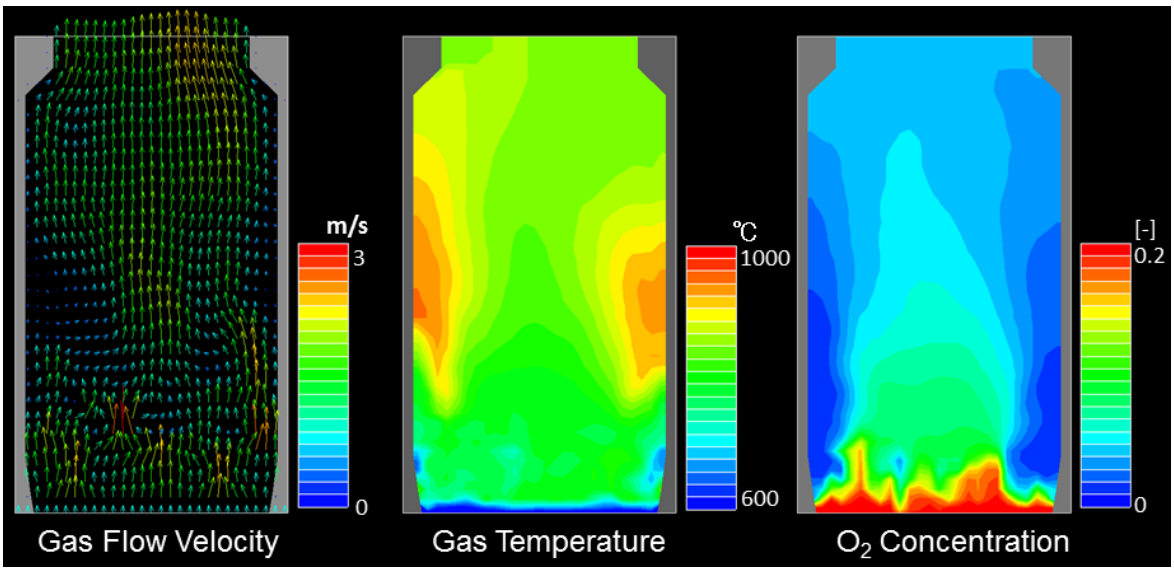


Concentration (volume fraction) distributions of reactive gases. In addition to oxygen (O_2), water vapor (H_2O) and carbon dioxide (CO_2), concentrations of combustible gases such as carbon monoxide (CO), methane (CH_4) and hydrogen (H_2) are also simulated.

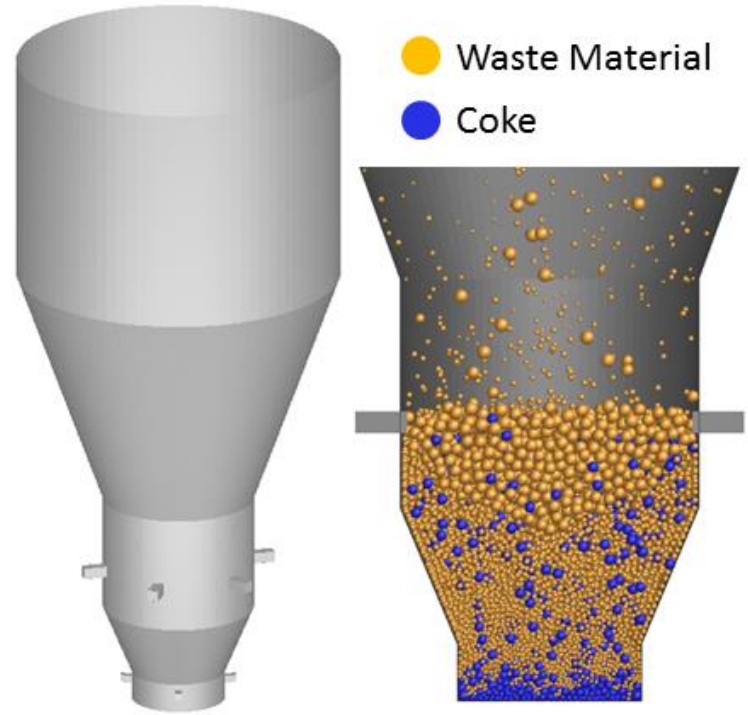
Combustion Simulation of Sludge in Fluidized Bed Incinerator

The combustion process of sludge, biomass and other fuel particles fed into a fluidized bed incinerator is represented by simulating the particle (sludge, sand) behavior, compressible gas flows, radiation fields and chemical reactions. The sludge combustion process is modeled in three stages: water evaporation, devolatilization (pyrolysis) and fixed carbon (char) combustion. The concentrations of reactive gases such as Oxygen (O_2), water vapor (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4) and hydrogen (H_2) produced and extinguished during the combustion process are also simulated numerically.

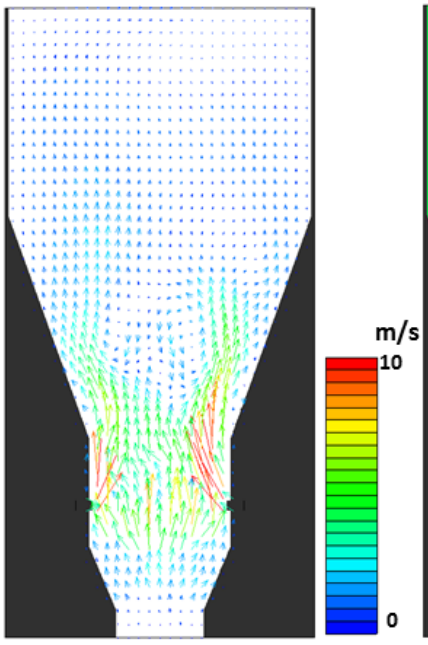




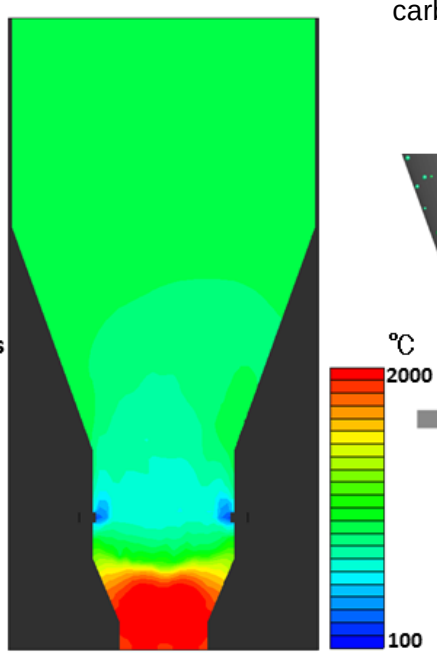
Combustion Simulation of Waste Material and Coke in Fluidized Bed Gasifier



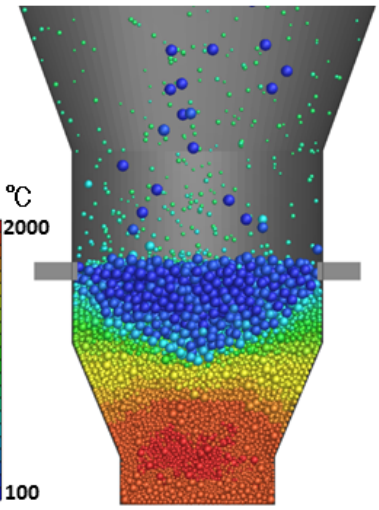
Combustion process of solid waste material and coke fed into a fluidized bed gasifier is simulated numerically. Combustible gases such as carbon monoxide, hydrogen and methane are produced in the gasification process. The combustion of solid waste particles is modeled in three stages: water evaporation, devolatilization (pyrolysis), and fixed carbon (char) combustion. Coke combustion, on the other hand, is simulated by modeling only fixed carbon combustion.



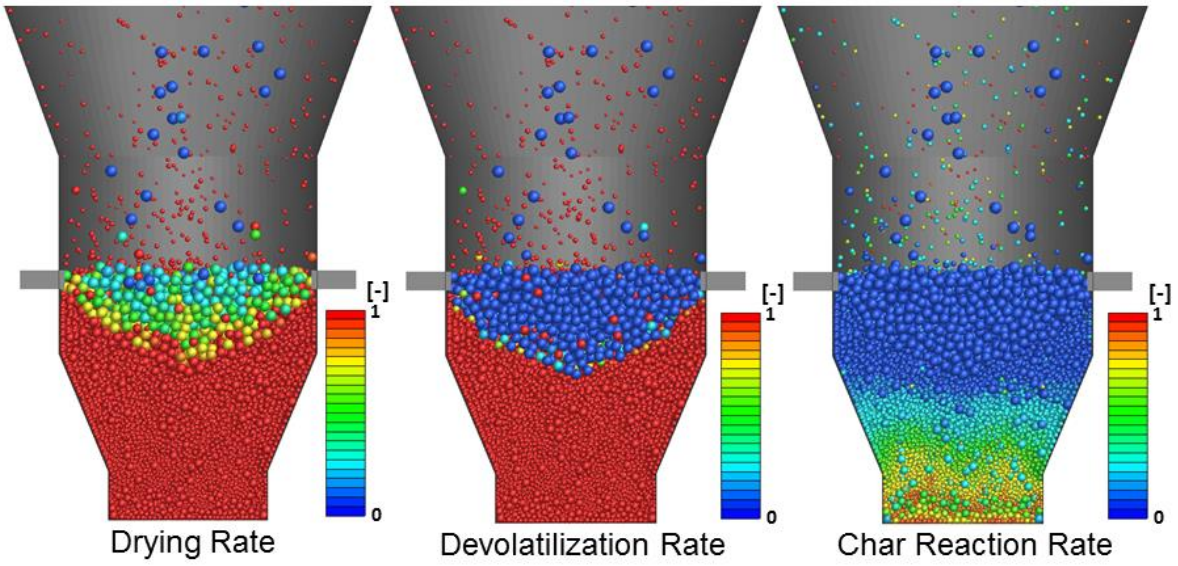
Gas Flow Velocity



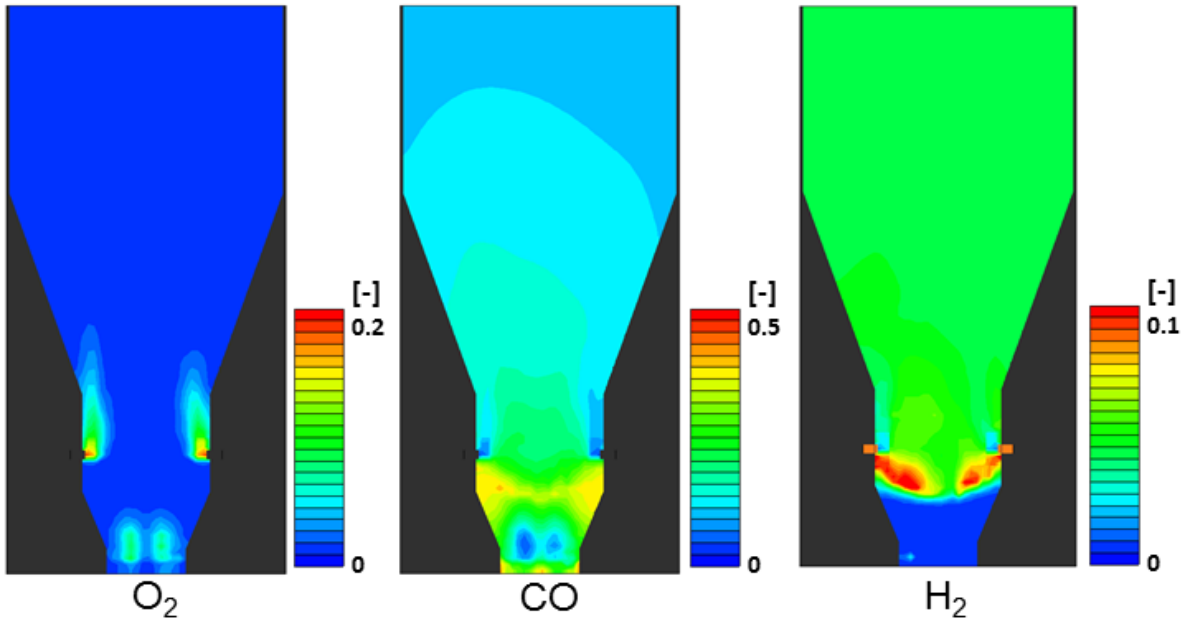
Gas Temperature



Particle Temperature

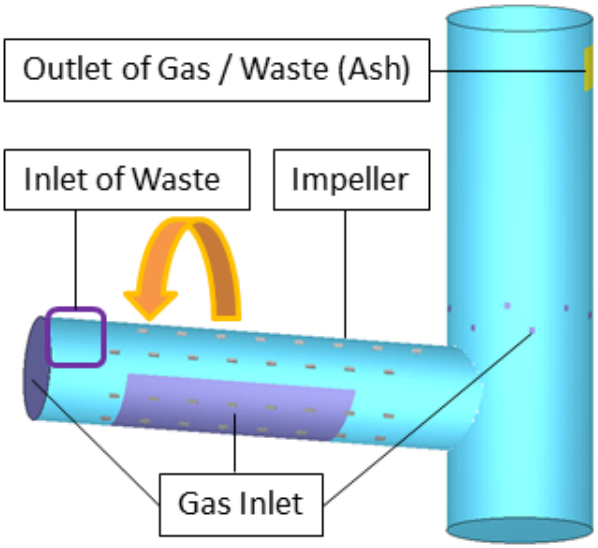


The combustion of solid waste particles is modeled in three stages: water evaporation, devolatilization (pyrolysis), and fixed carbon (char) combustion. Coke combustion, on the other hand, is simulated by modeling only fixed carbon combustion.

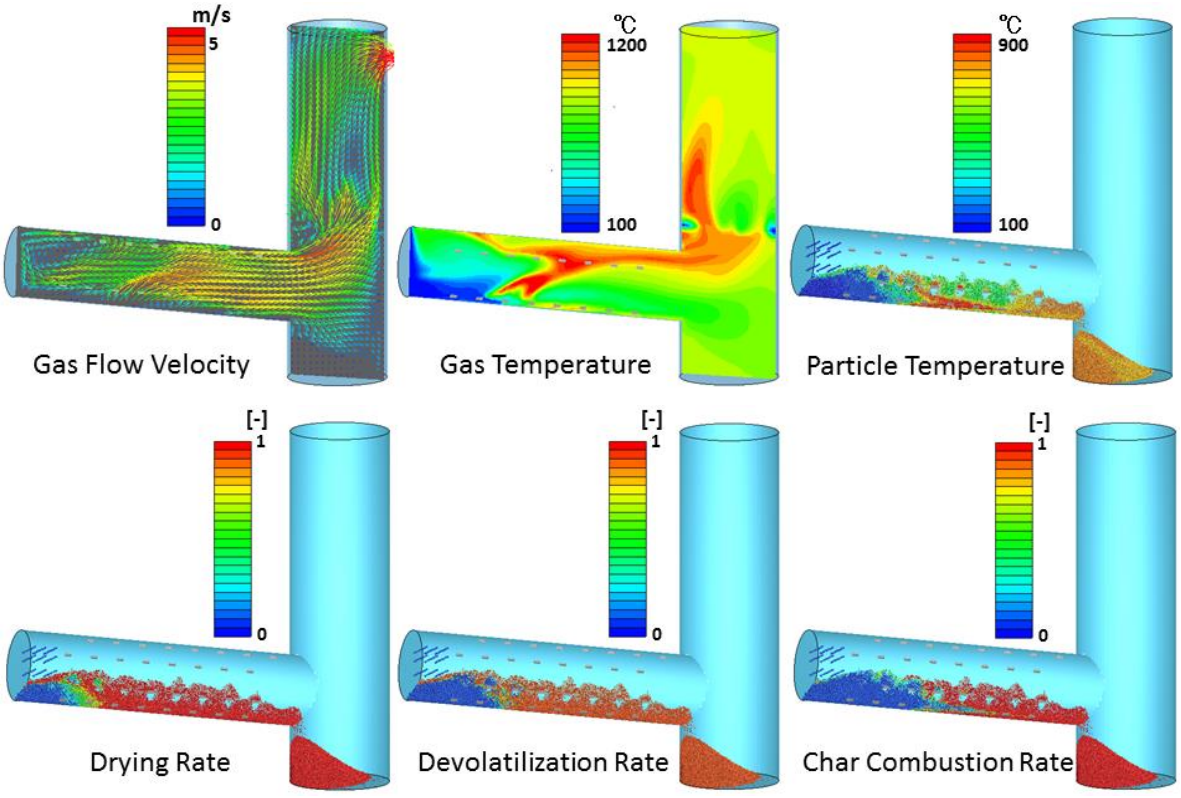


Concentration distributions of oxygen (O_2) and combustible gases. The combustible gases such as carbon monoxide (CO), hydrogen (H_2), and methane (CH_4) are produced in the gasification process.

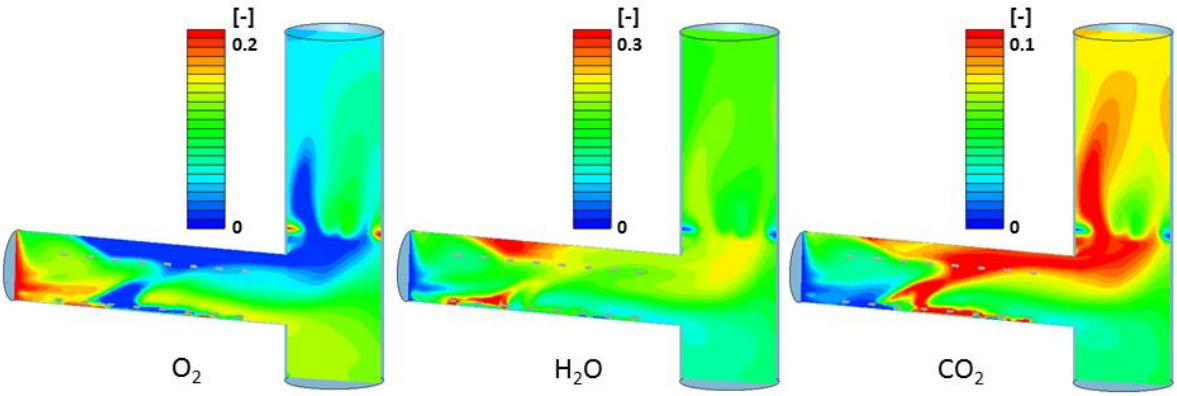
Combustion Simulation of Waste in Rotary Kiln Incinerator



The combustion process of solid waste fed into a rotary kiln incinerator is represented by simulating the behavior of solid waste particles, compressible flows of reactive gases, radiation fields, and combustion reactions. The combustion process of solid waste particles is modeled in three stages: water evaporation, devolatilization (pyrolysis), and combustion of fixed carbon (char). The concentrations of reactive gases such as Oxygen (O_2), water vapor (H_2O), carbon dioxide (CO_2), carbon monoxide (CO), methane (CH_4), hydrogen (H_2) produced and extinguished in the combustion process are also simulated simultaneously.



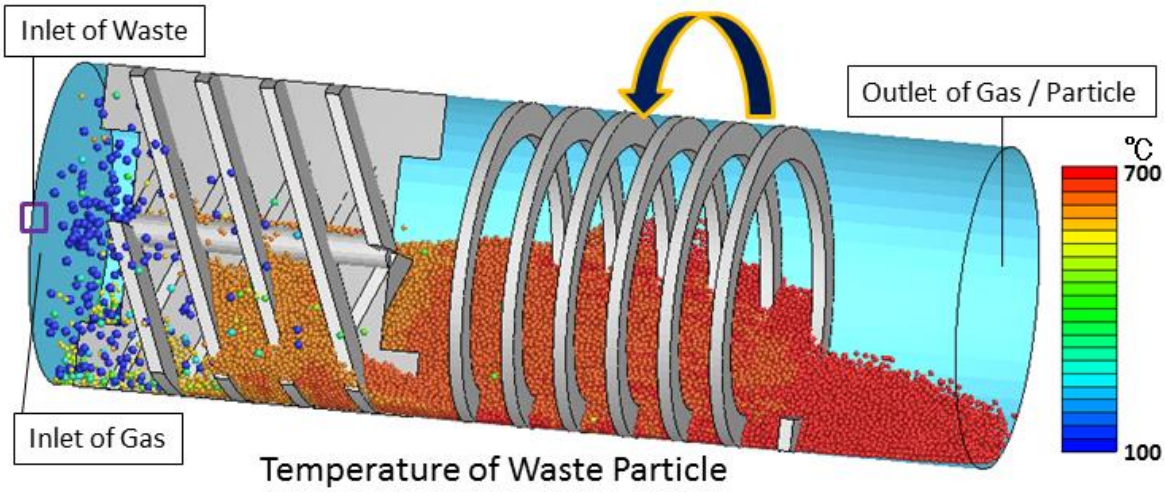
The combustion process of the solid waste particles is simulated in three stages: water evaporation, devolatilization (pyrolysis) and fixed carbon (char) combustion.

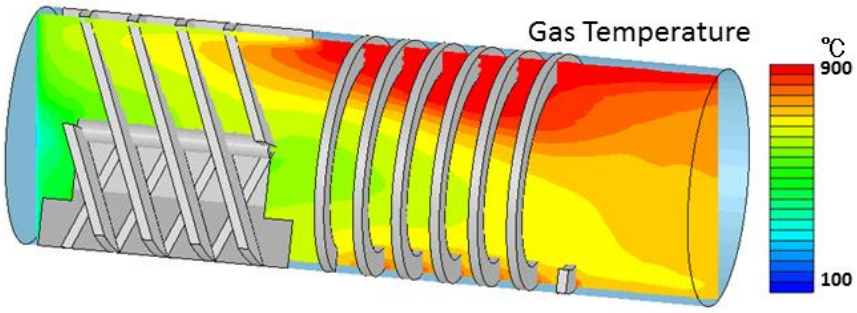


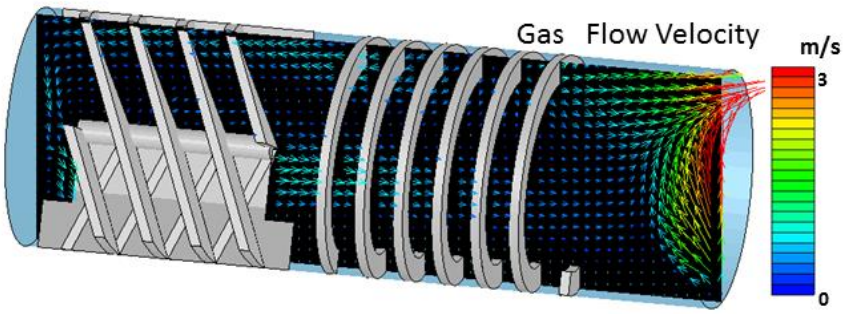
Concentration (volume fraction) distributions of reactive gases. In addition to oxygen (O2), water vapor (H_2O) and carbon dioxide (CO_2), combustible gases such as carbon monoxide (CO), methane (CH_4) and hydrogen (H_2) are also simulated numerically.

Gasification Simulation of Waste in Rotary Kiln
Pyrolysis Gasification Reforming Furnace

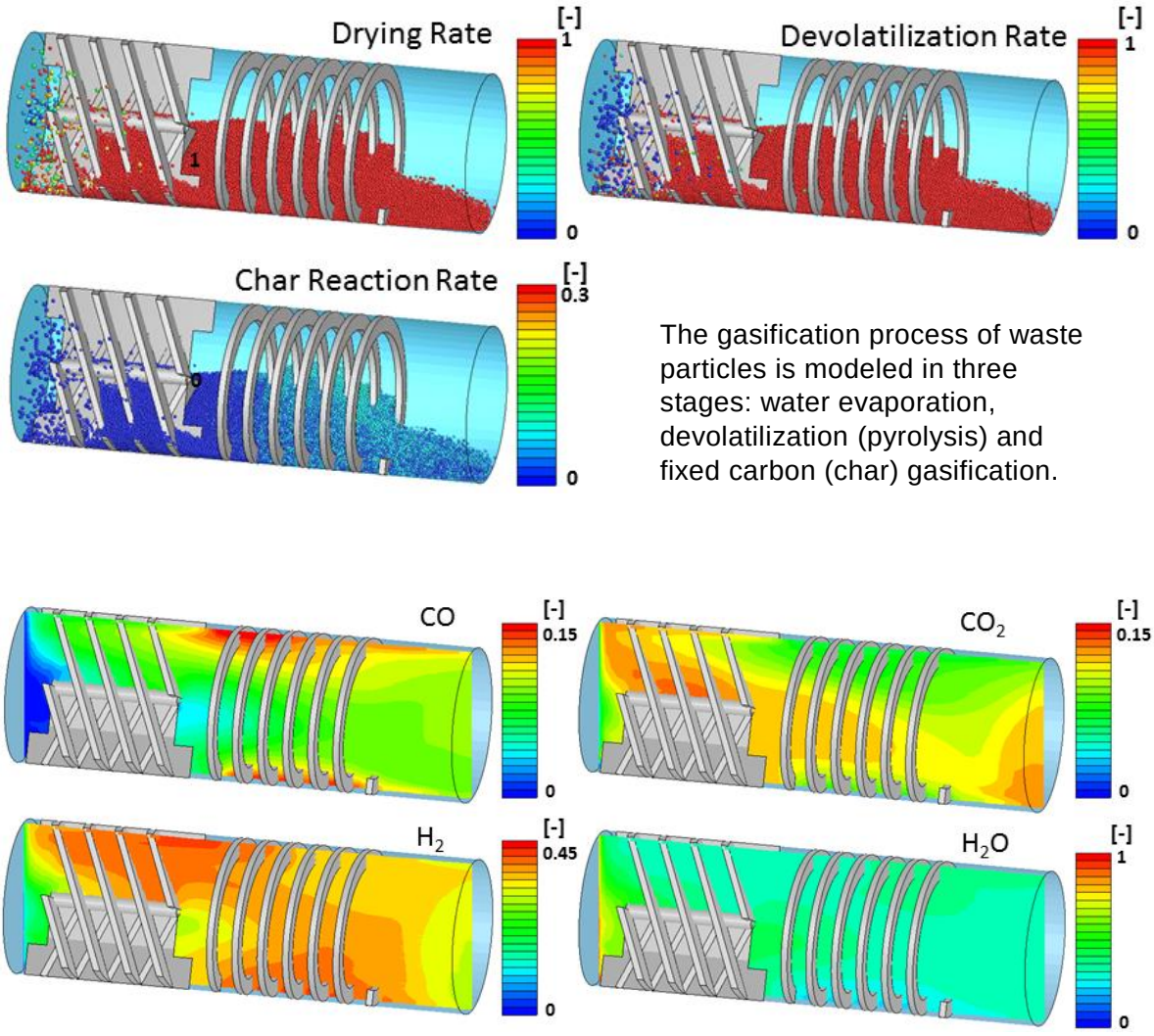
Numerical simulation of gasification process of waste material fed into a rotary kiln pyrolysis gasification reforming furnace.







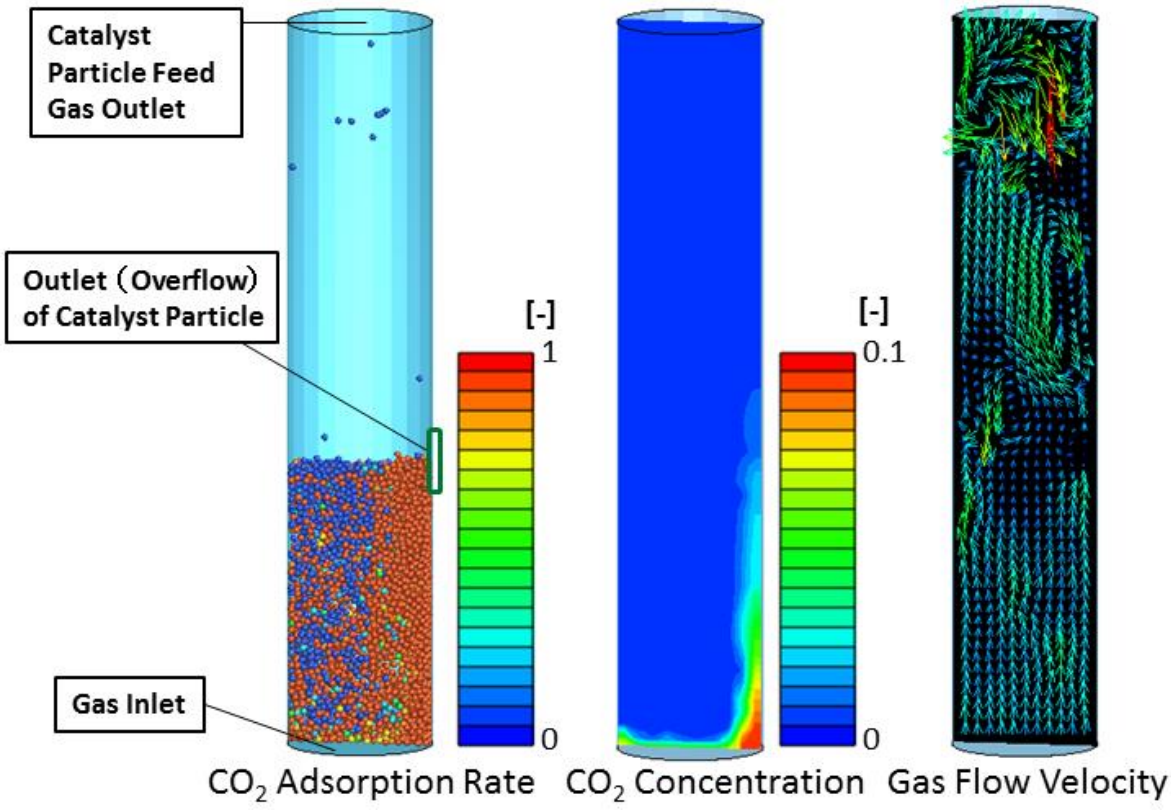
Gasification process is represented by simulating the behavior of solid waste particles, compressible flows of reactive gases, radiation fields and gasification reactions. The gasification process of solid waste particles is modeled in three stages: water evaporation, devolatilization (pyrolysis), and fixed carbon (char) gasification. In addition, the concentrations of carbon monoxide (CO), water vapor (H_2O), carbon dioxide (CO_2), methane (CH_4) and hydrogen (H_2), which are produced and extinguished during gasification, are also simulated numerically.



Concentration (volume fraction) distributions of reactive gases. In addition to the above concentration components, methane (CH_4) is also simulated.

CO_2 Adsorption Simulation in Fluidized Bed Reactor

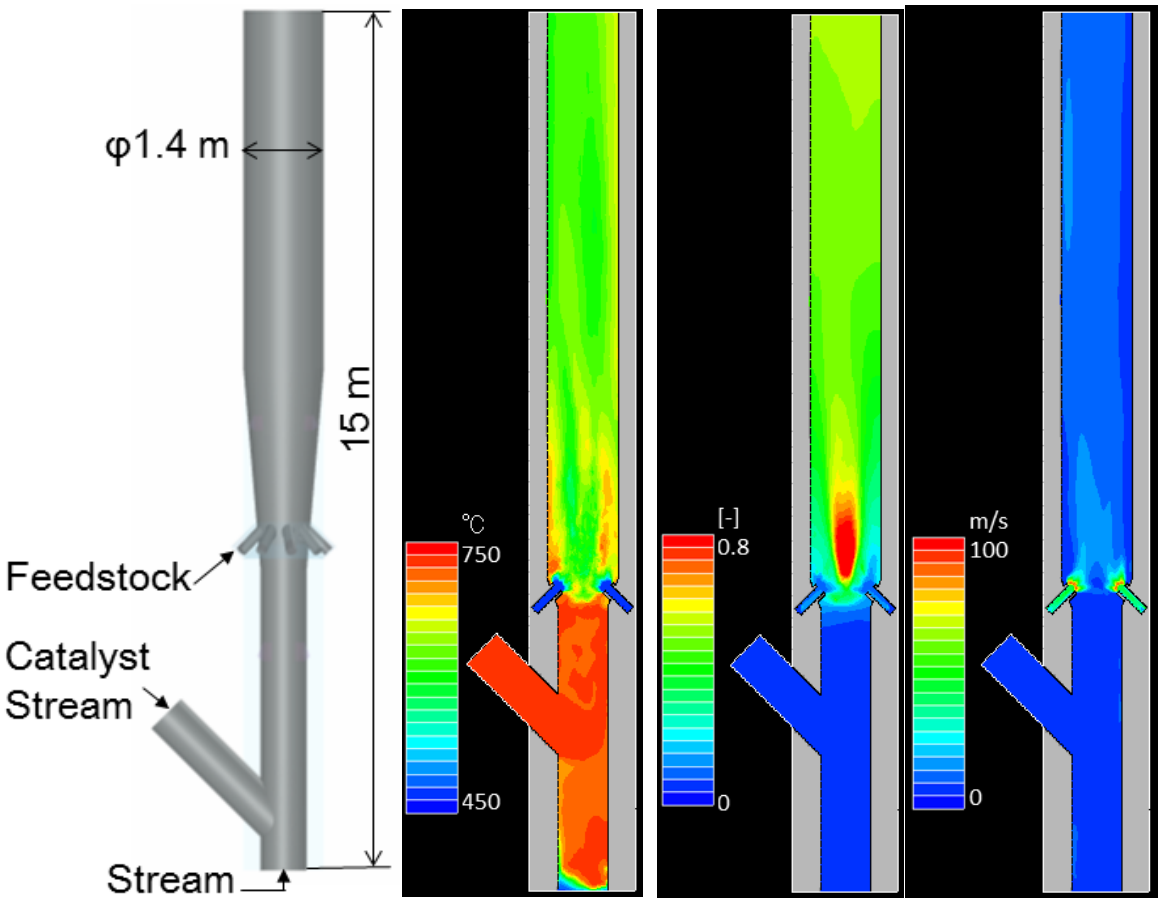
The reaction process in which carbon dioxide (CO_2) contained in the gas is adsorbed onto the catalyst particles is numerically simulated by feeding the gas into a fluidized bed filled with catalyst (Na_2O) particles.



From left to right: carbon dioxide (CO_2) adsorption rate of the catalyst (Na_2O) particles, carbon dioxide (CO_2) concentration in the gas and gas flow velocity distribution. The CO_2 adsorption rate when the catalyst particles are fed is 0.

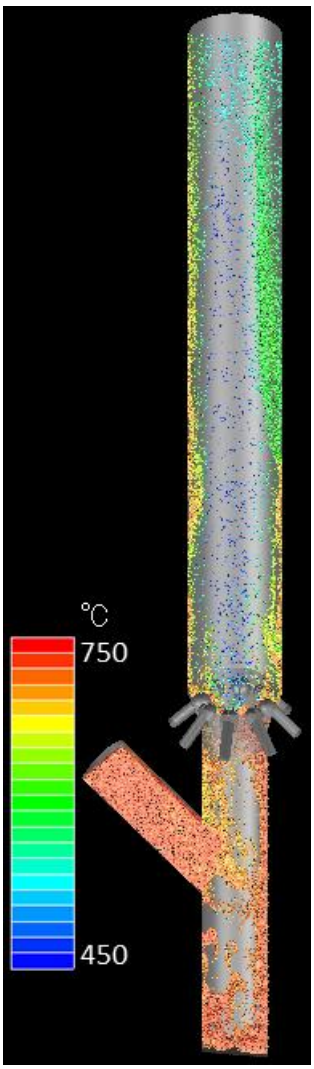
Numerical Simulation of Catalytic Particle Behavior and Droplet Evaporation in FCC Reactor

The compressible gas flow, catalyst particle behavior, and droplet evaporation process in a Fluidized Catalytic Cracking (FCC) reactor are represented by numerical simulation. The heat and radiation fields are also simulated.

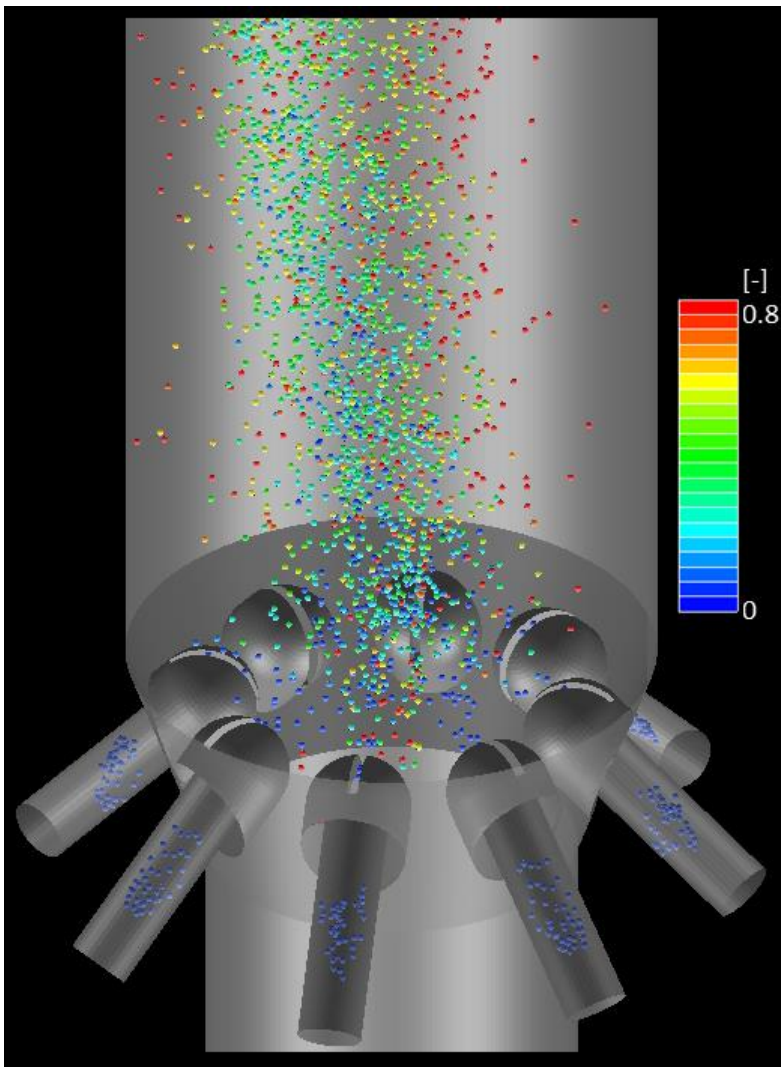


Gas Temperature | Water Vapor Concentration | Absolute Value of Gas Flow Velocity

The DEM-based representative particle model is used to simulate behaviors of catalyst particles and liquid droplets. Both the representative particle diameter (particle diameter used for the calculation of particle contact) and real particle diameter decrease as the particle mass decreases due to evaporation of the liquid. The real particle diameter is used to calculate the catalyst particle and droplet behavior, the radiation field, particle-fluid drag force, particle-fluid heat transfer, particle reaction surface area, and so on. Evaporative gases are produced during the evaporation process.



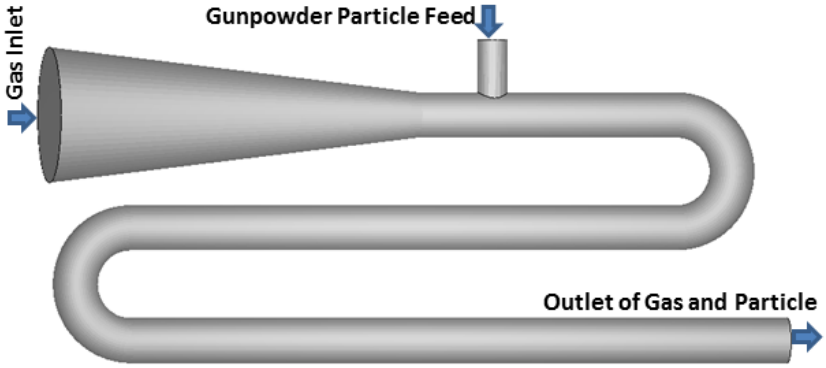
Catalytic Particle Temperature



Droplet Evaporation Rate

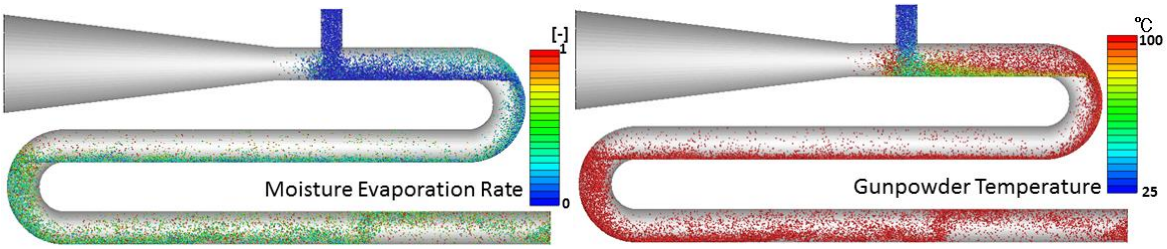
The evaporation rate of the liquid is calculated on the assumption that after the temperature of the droplet particles reaches the boiling point, the amount of heat received by the particles from the hot gas due to particle-fluid heat transfer is converted into vaporization heat.

Numerical Simulation of Gunpowder Drying Process

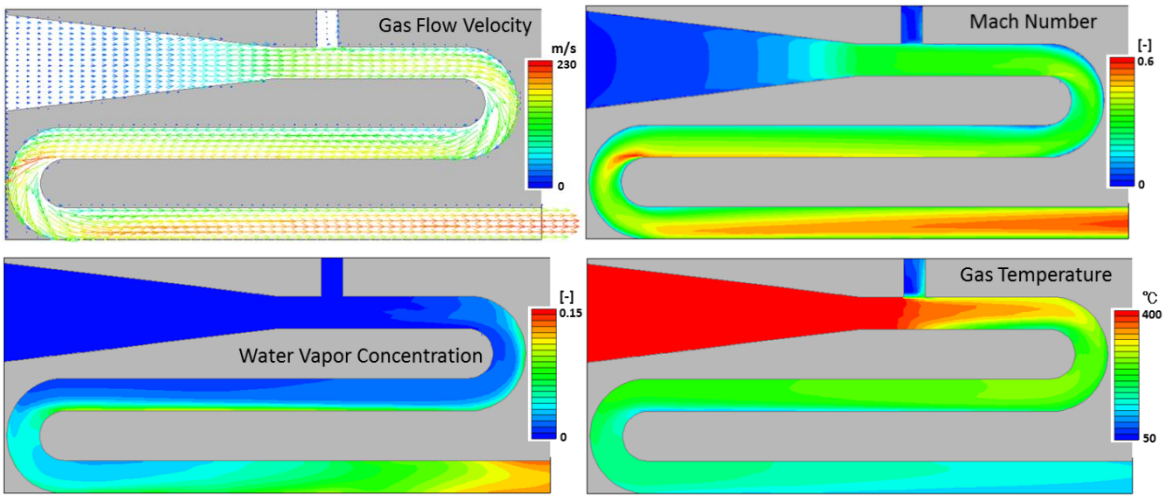


The process of evaporation of water contained in gunpowder is numerically simulated when the gunpowder particles are injected into a high speed, hot compressible gas flow.

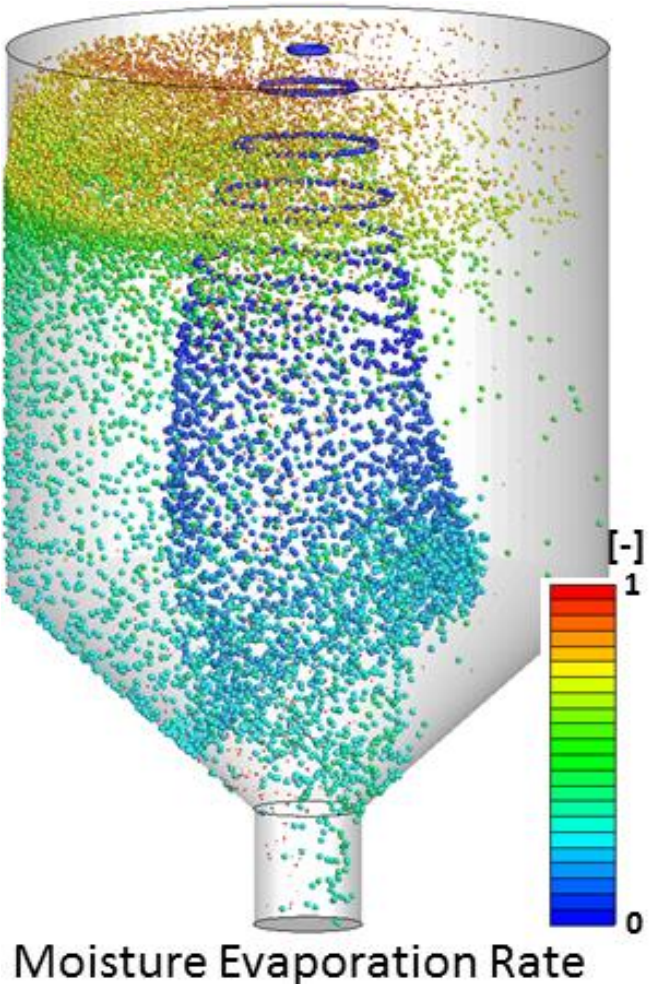
The DEM-based representative particle model is used to simulate gunpowder particles, and the real particle size at the time of particle injection is simulated by specifying the particle size distribution. The simulation is carried out in such a way that the particle density of the representative particle diameter (particle diameter used for the calculation of particle contact) diameter and the real particle diameter decreases according to the decrease in the particle mass due to the evaporation of water. The actual particle diameter is used in the simulation of particle behavior, temperature, particle-fluid drag force, particle-fluid heat transfer, particle surface area, and so on. In the figures below, gunpowder particles are twice the size of the representative particles.



The water evaporation rate is calculated on the assumption that after the particle (liquid) temperature reaches the boiling point (100°C), the amount of heat received by the particles from the hot gas by particle-fluid heat transfer is converted to vaporization heat. Water vapor is produced during evaporation process.



Droplet Evaporation Simulation in Spray Dryer

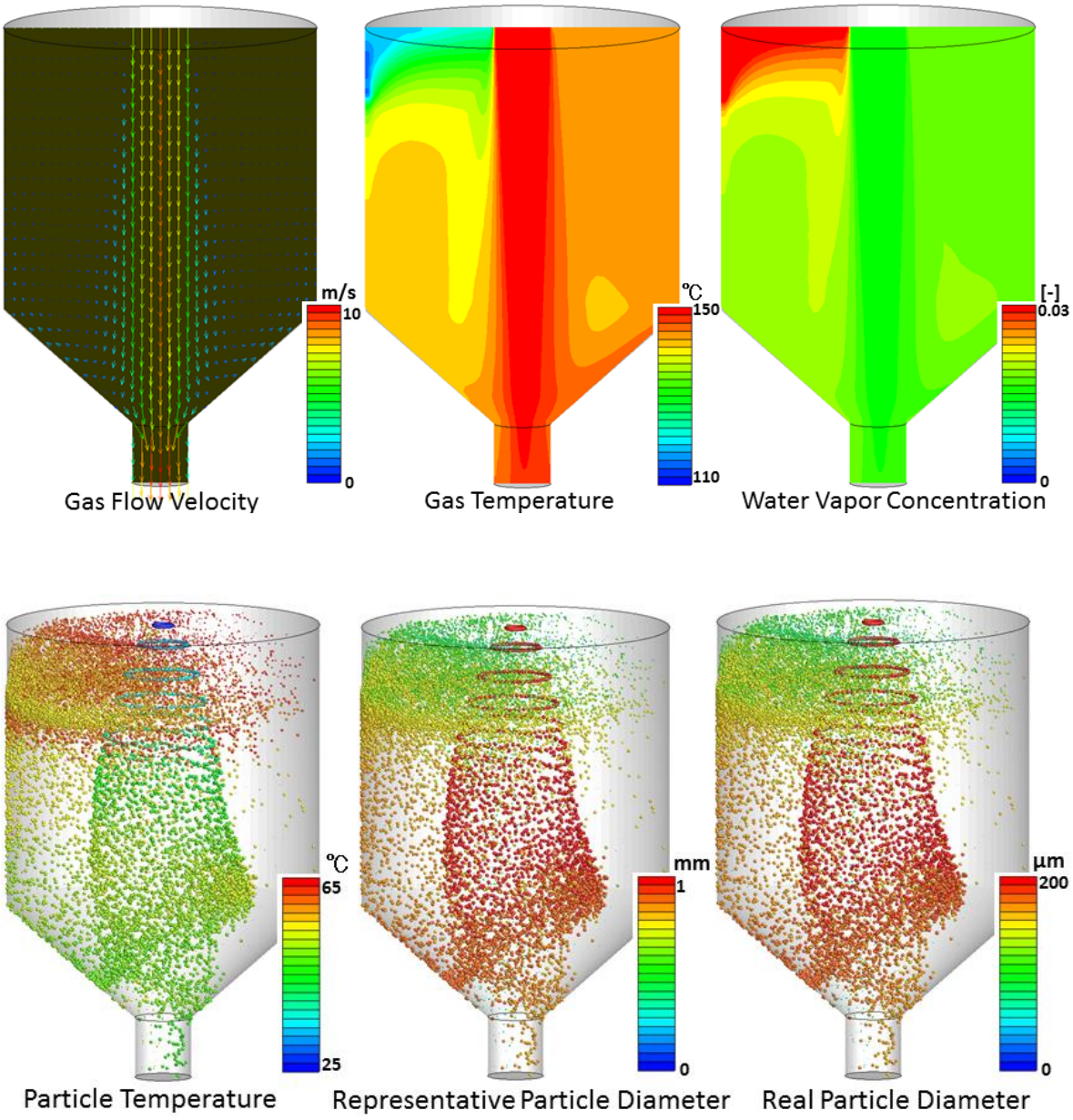


The process of evaporation of liquid droplets injected with gas from a rotating nozzle located in the center near the ceiling of the spray dryer is simulated numerically.

In addition to evaporation due to boiling after the droplet reaches the boiling point (100 °C), evaporation at room temperature before reaching the boiling point is also considered as a liquid evaporation model. For evaporation at temperature before reaching the boiling point, the evaporation rate is determined using an evaporation model based on the water vapor concentration in the gas and the saturated vapor pressure.

In the simulation, particles are assumed to be droplets without solids, but it is also possible to assume that the liquid adheres to the solid particle surface.

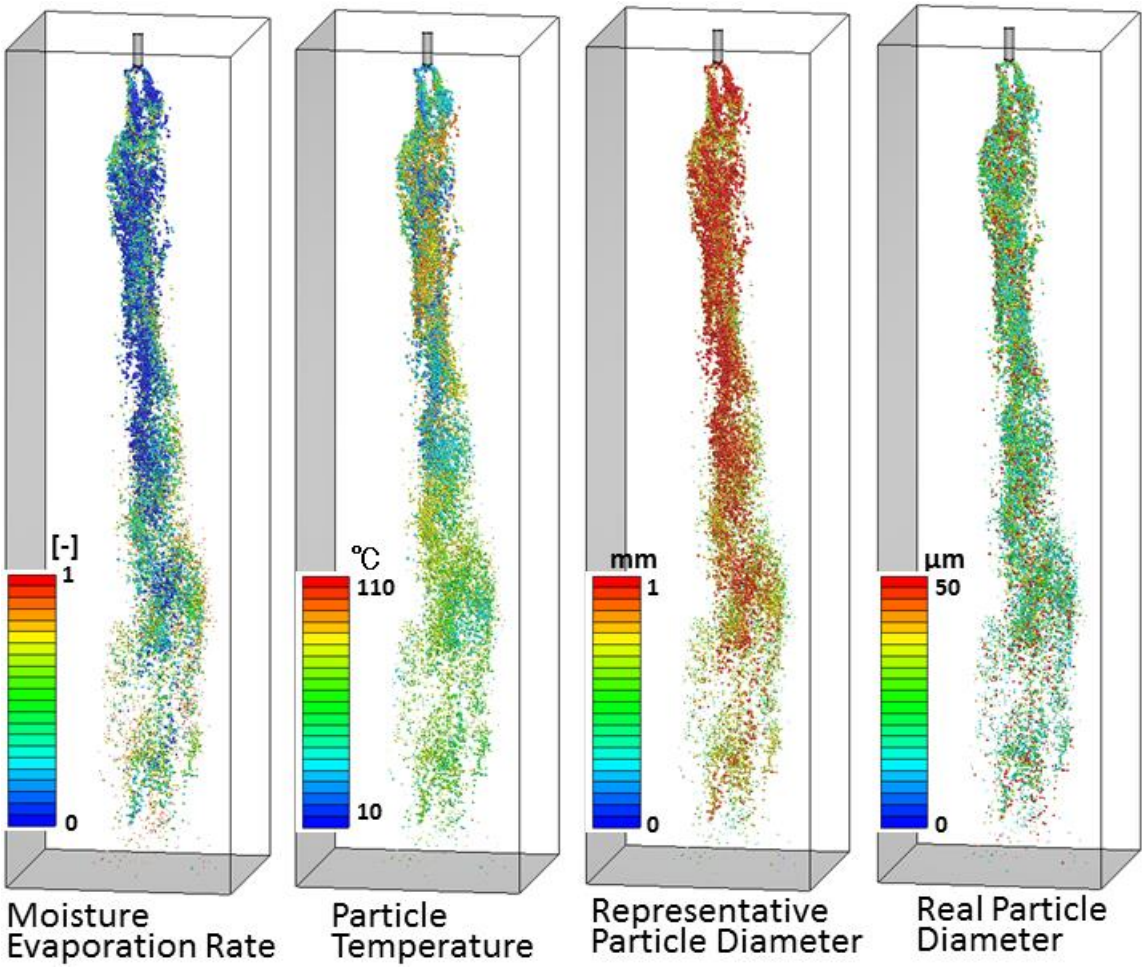
In the figure above, the droplet is 20 times larger than the representative particle diameter (particle diameter used for the calculation of particle contact).

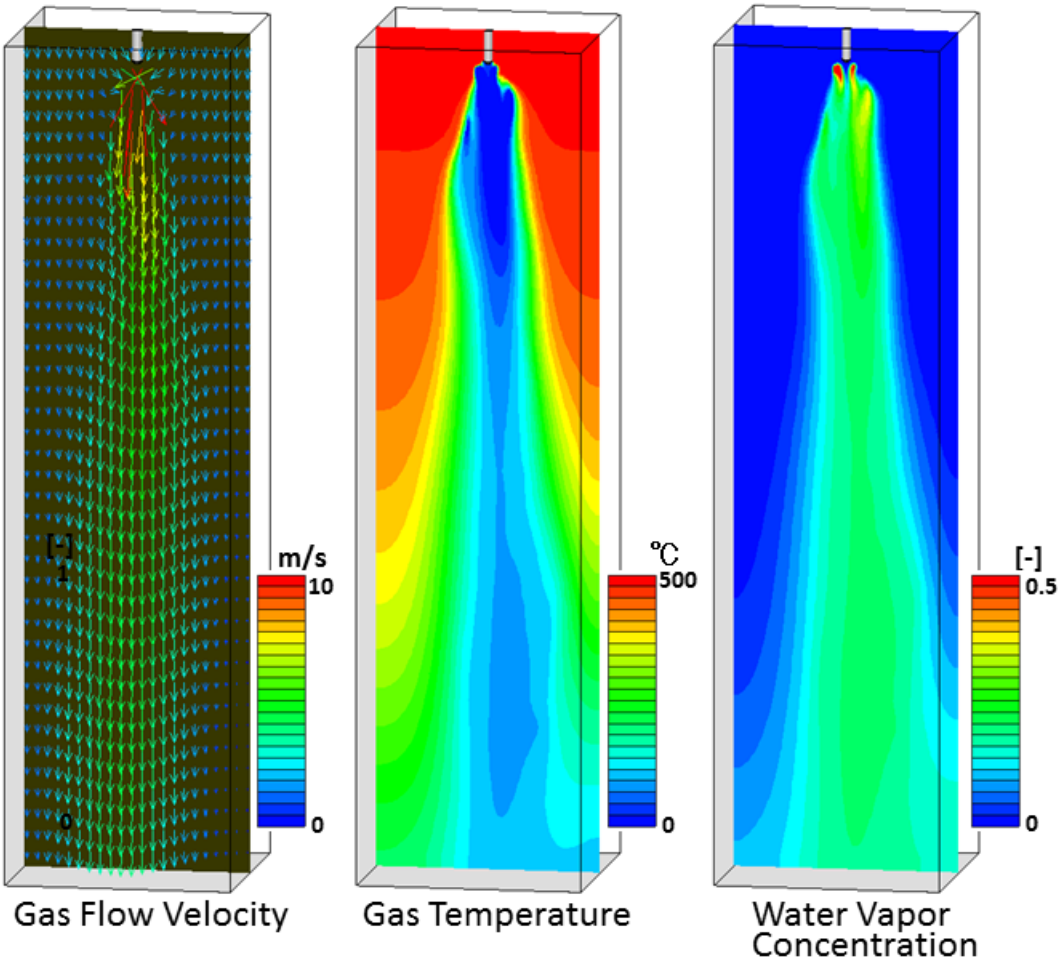


The DEM-based representative particle model is used for the simulation of the droplet particles, giving a diameter distribution for the real droplet particles at the time of generation. Both the representative particle and real particle diameters decrease as the particle mass decreases with evaporation of the liquid. The real particle diameter is used for the calculation of particle-fluid drag force, particle-fluid heat transfer and particle surface area, which are related to droplet behavior, temperature and evaporation rate. In the figure above, the droplet is shown at 20 times larger than the representative particles.

Evaporation Simulation of Droplet Sprayed from Nozzle

The process of evaporation of fine droplets sprayed from the nozzle at the top of the device is so. Gas is also ejected from the vicinity of the nozzle to atomize the droplets.
The DEM-based representative particle model is used to simulate droplet particles, giving a particle diameter distribution for the real particles at droplet generation. Both the representative particle diameter (particle diameter used for the calculation of particle contact) and the real particle diameter decrease as the particle mass decreases with evaporation of the liquid. The real particle diameter is used for the calculation of particle-fluid drag force, particle-fluid heat transfer and particle surface area, which are related to droplet behavior, temperature and evaporation rate.
In addition to evaporation due to boiling after the droplet reaches the boiling point (100 °C), evaporation at room temperature before reaching the boiling point is also considered as a liquid evaporation model. For evaporation at temperature before reaching the boiling point, the evaporation rate is determined using an evaporation model based on the water vapor concentration in the gas and the saturated vapor pressure.
In the figure below, the droplet size is 10 times larger than the representative particle diameter used in the simulation.



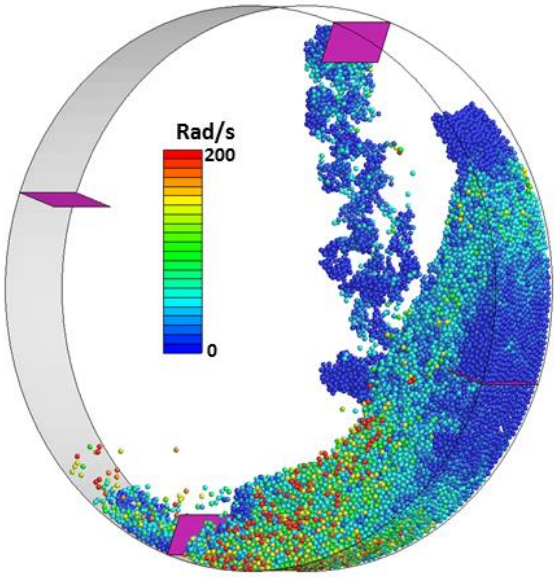


Gas flow velocity, gas temperature and water vapor concentration in a vertical section.

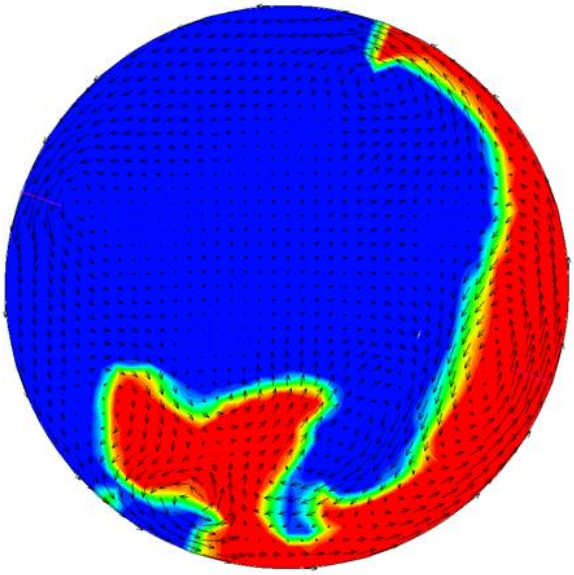
Gas is emitted from the vicinity of the nozzle to atomize the droplets. As the liquid evaporates, water vapor is produced.

Simulation of Liquid Flow and Ball Behavior in Wet Ball Mill

Liquid flow and ball behavior in a wet ball mill are simulated numerically. The liquid flow is simulated using the VOF (Volume-of-Fluid) method. On the other hand, the behavior of ball particles with a diameter of 2 mm is simulated by DEM (Discrete Element Method). For particles that have been flew out of the liquid (into the air), the liquid bridge force (adhesion force) is taken into account in DEM simulation, assuming that the liquid adheres to the particle surface. For particles within the liquid, no liquid bridge force acts.



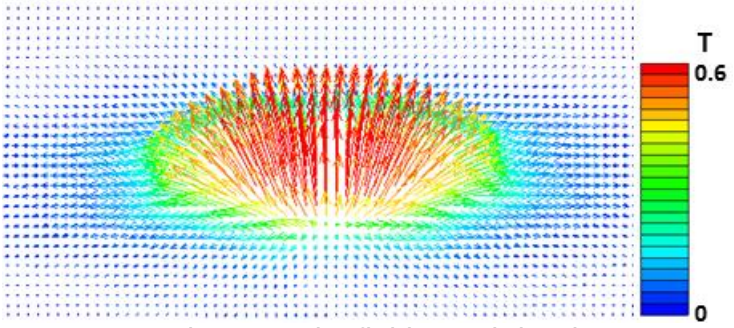
Behavior of ball particles.
Particle display color corresponds to the rotational angular velocity.



Distributions of Liquid volume fraction and liquid flow velocity at the center section of the mill.

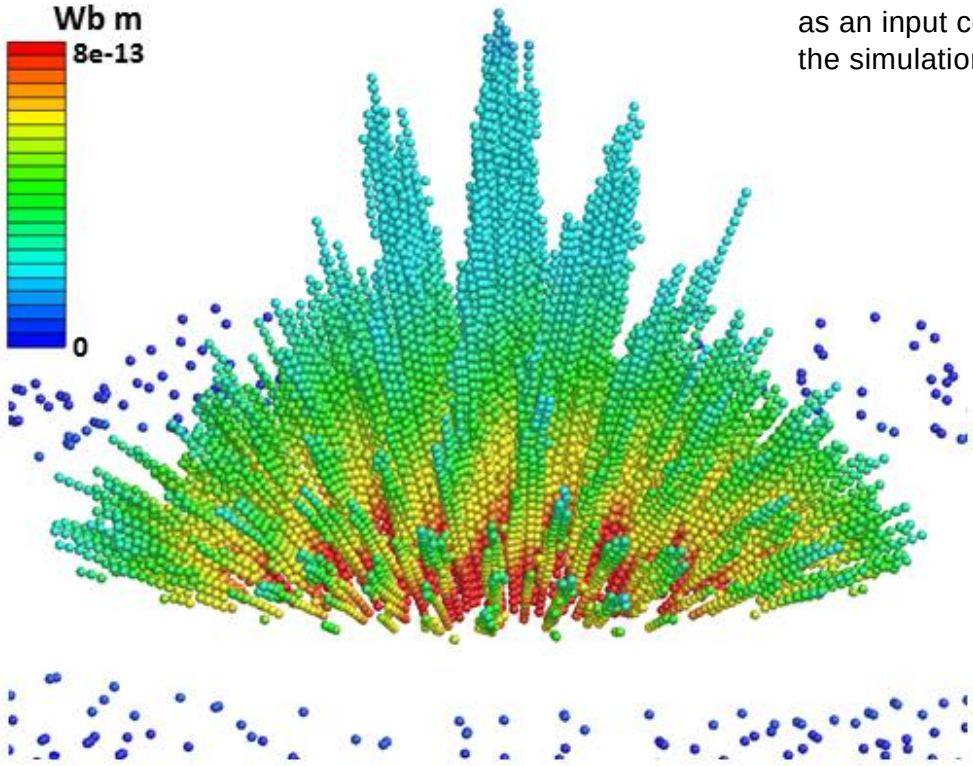
Numerical Simulation of Magnetic Particle Behavior in External Magnetic Field

It is known that a magnetic brush is formed by the magnetic force acting on the particles when magnetic particles such as toner are dispersed in an external magnetic field. Assuming an infinitesimal magnetic dipole at the particle center, we calculate the magnetic force acting on the magnetic particle as the force acting on the magnetic dipole. The magnetic particle behavior is simulated by the DEM-based representative particle model.



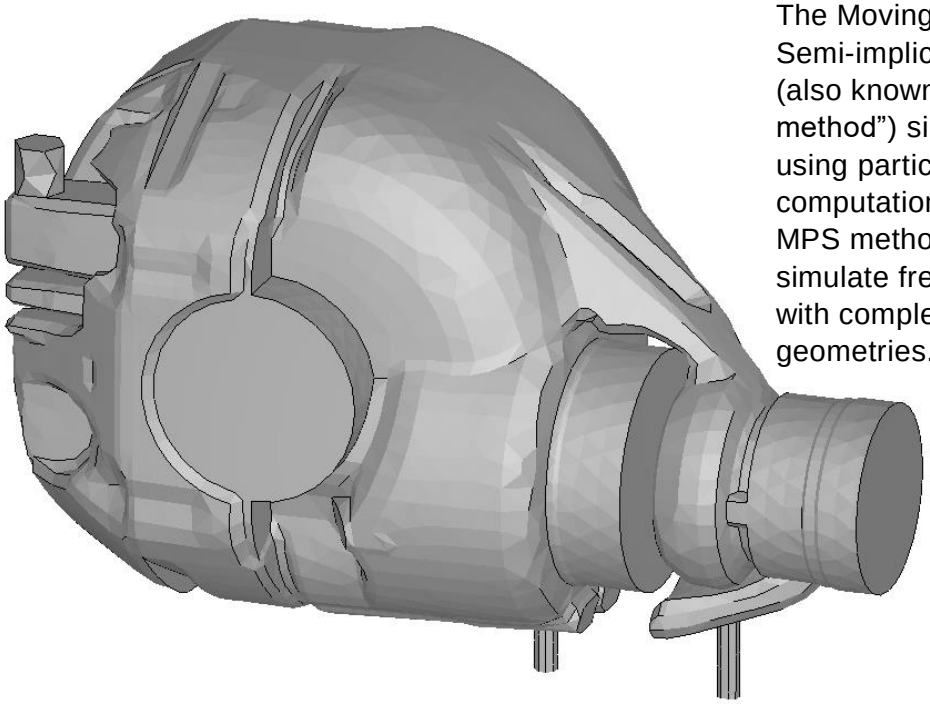
External magnetic field used in the magnetic particle behavior simulation

In the figure below, magnetic particles with a real particle diameter of 3.36 μm are simulated numerically by the representative particle model using representative particles with a diameter of 500 μm. The external magnetic field (left figure) is given as an input condition for the simulation.

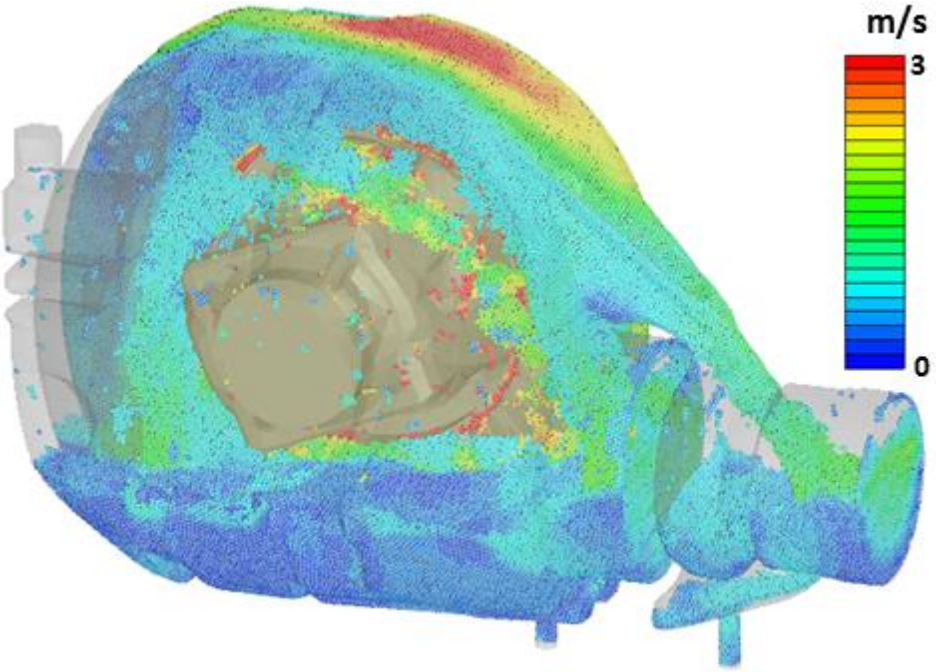


Behavior of magnetic particles in an external magnetic field. The particle display color represents the magnetic dipole moment.

Liquid Behavior Simulation in Final Drive by MPS method



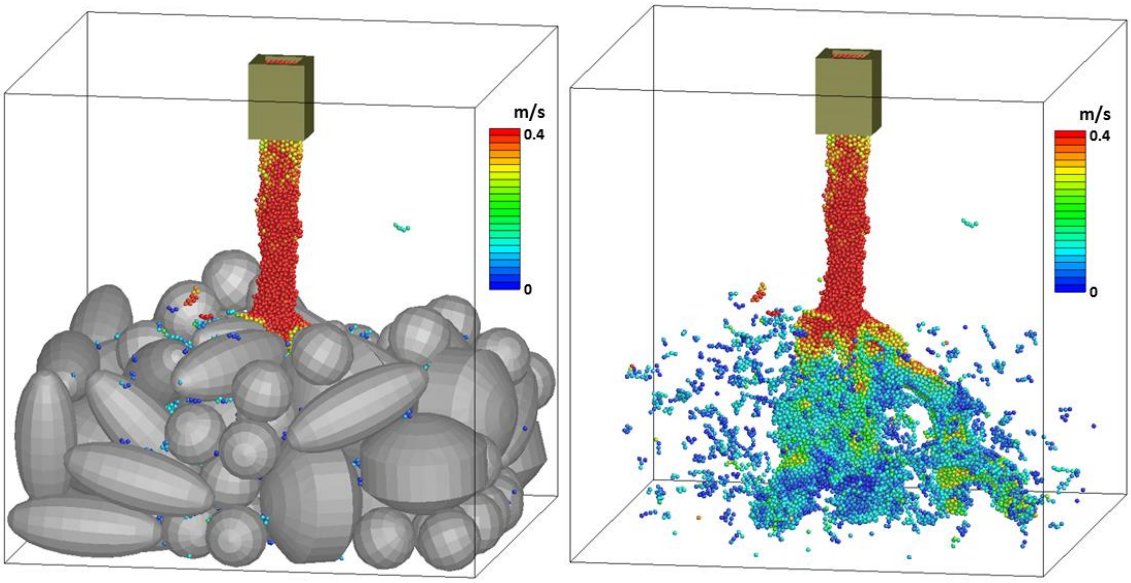
The Moving Particle Semi-implicit (MPS) method (also known as “particle method”) simulates the flow using particles instead of computational grids The MPS method can be used to simulate free surface flows with complex free surface geometries.



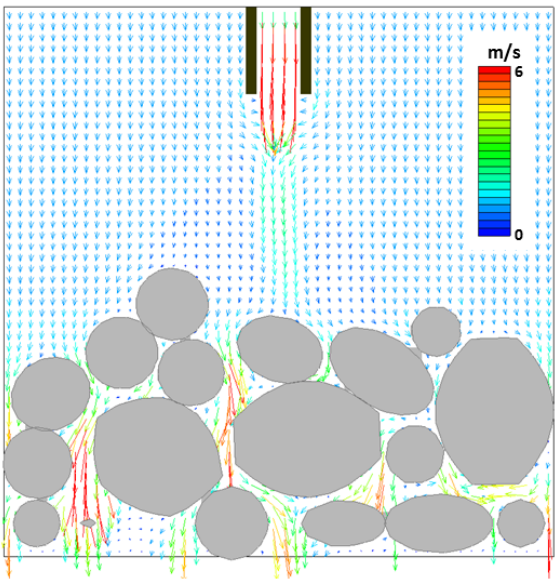
Liquid flow at a given moment. The MPS particle display color represents the absolute value of liquid velocity.

Liquid and Gas Flow Simulation in Trickle Bed Reactor

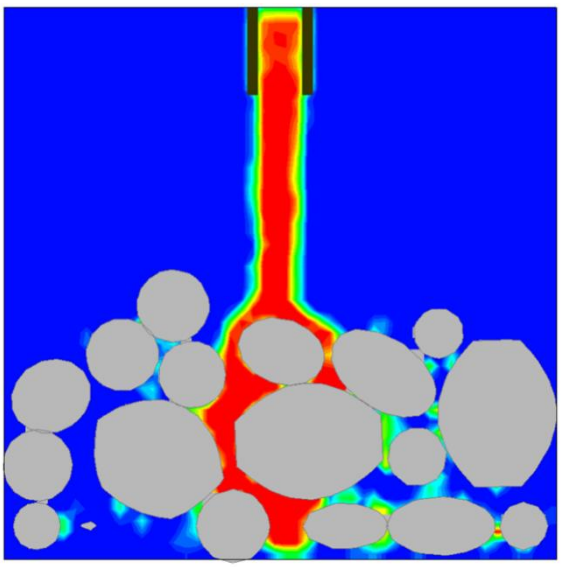
The liquid flow in a trickle bed reactor filled with catalyst particles of various shapes is simulated numerically by the MPS (Moving Particle Semi-implicit) method. The gas flow is simulated by the finite difference (volume) method using computational grids.



Distribution of liquid flow velocity passing between catalyst particles. Particle display color represents the absolute value of MPS particle velocity.



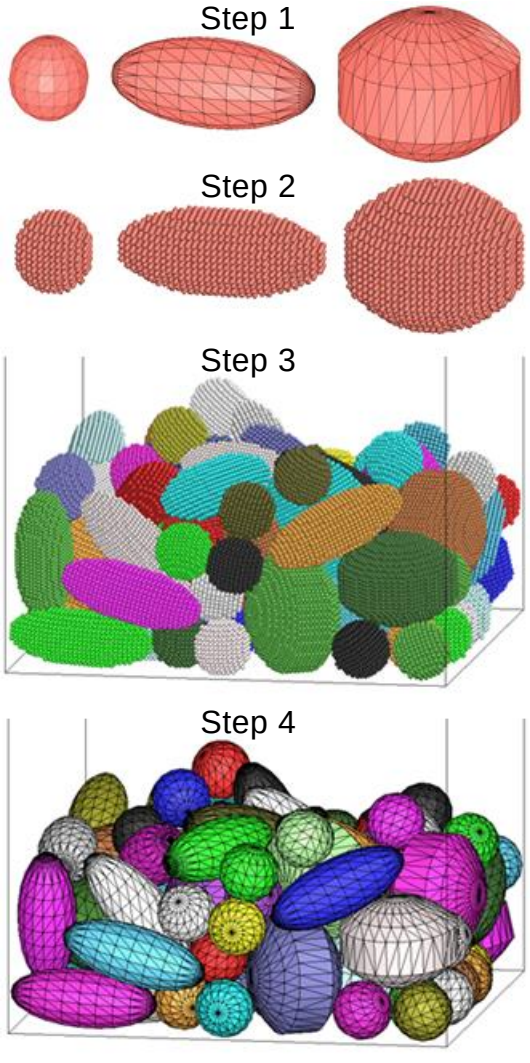
Gas flow velocity distribution in the central section of the reactor. Gas flows in from the top front.



Contour of the liquid distribution in the central section of the reactor calculated from the MPS particle arrangement.

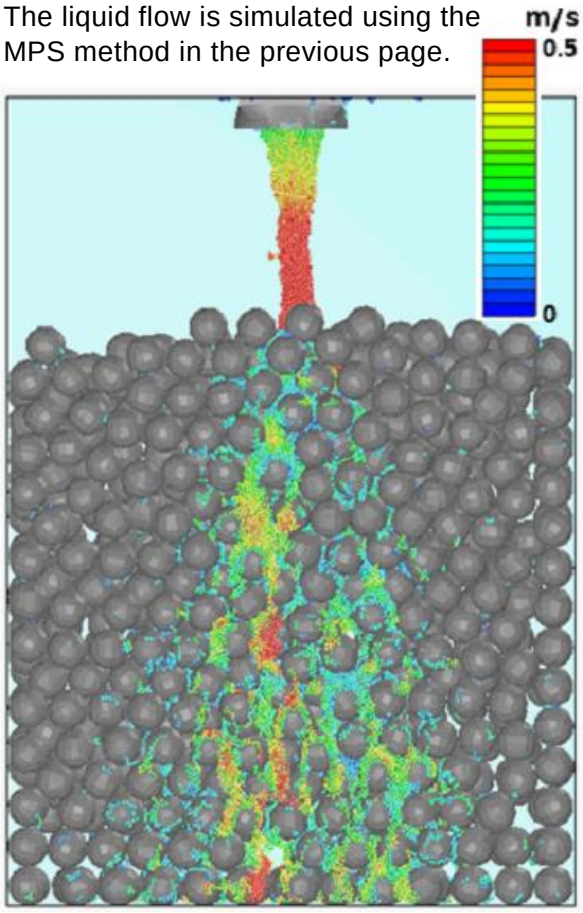
Simulation procedure for trickle-bed reactors

Prior to performing flow simulations in a trickle-bed reactor, it is necessary to reproduce packing conditions of the catalyst particles. Since the catalyst particles have a variety of shapes, the DEM simulation should be performed in several steps using combined particles created from CAD geometry data.



Computational results for the liquid flow using the MPS method described in the previous page.

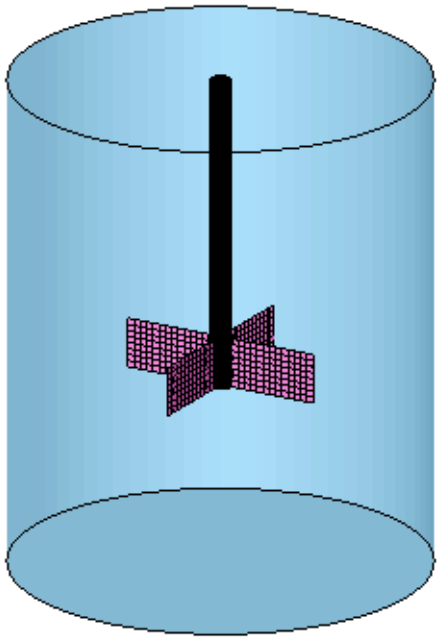
Step 1:
Create catalyst particles of various shapes as wall elements. Wall elements can be created from the RFLOW pre or CAD via STL files.
Step 2:
Generate combined particles within each wall element. Combined particles can be generated by the RFLOW solver.
Step3:
Perform free-fall DEM simulation using the combined particles until all the particles are stationary.
Step4:
Restore the corresponding wall elements from the stationary combined particles with the RFLOW solver.
Step5:
The liquid flow is simulated using the MPS method in the previous page.



Liquid flow in a trickle bed reactor filled with spherical catalyst particles obtained by the MPS method simulation.

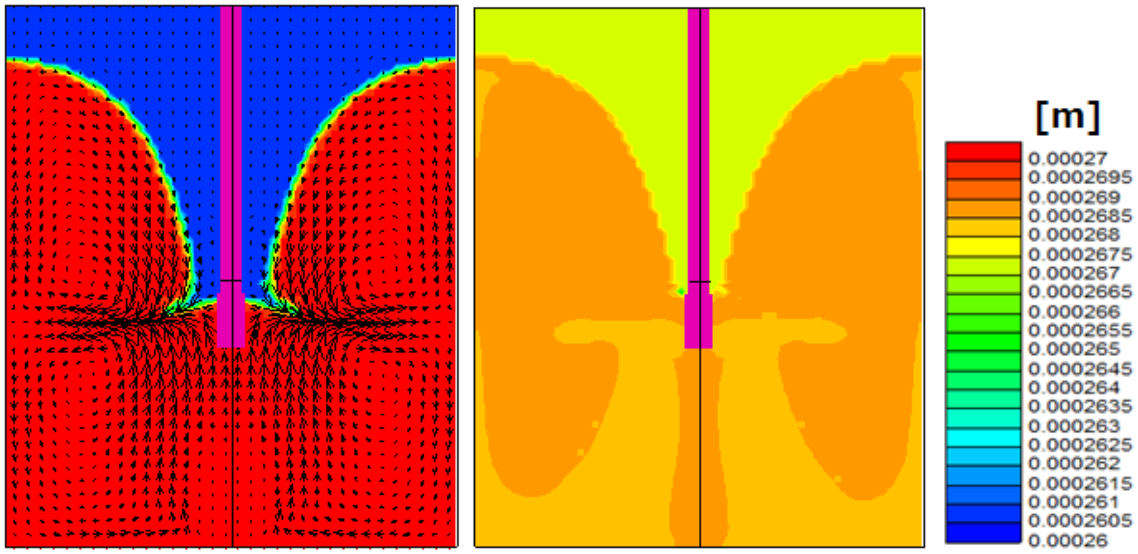
Simulation of Droplet Breakup and Coalescence in Agitated Tank

Liquid-liquid dispersed system multiphase flow is simulated numerically, considering the breakup and coalescence of droplets in an agitated tank.



The 14-fluid (continuous phase + 13 dispersed phases) Euler-Euler multiphase flow model, in which the droplets are approximated by the continuum and divided into 13 dispersed phases of different droplet diameters..

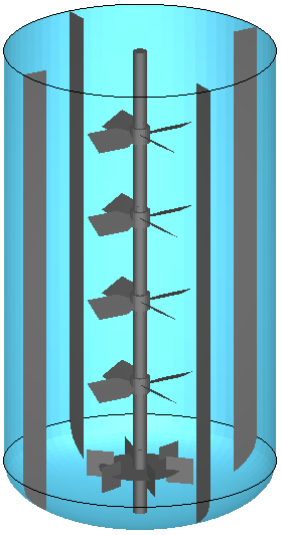
As for the droplet breakup model, the maximum stable droplet diameter is determined by the shear stress in the turbulent flow field, similar to the bubble breakup model. On the other hand, the coalescence is simulated using an RFLOW's original coalescence model, in which the coalescence condition is determined by the Weber number based on the velocity difference of the contacting droplets. As the droplets breakup or coalesce, they move to another dispersed phase at the same location with a different droplet diameter, thereby obtaining the droplet diameter distribution for each location.



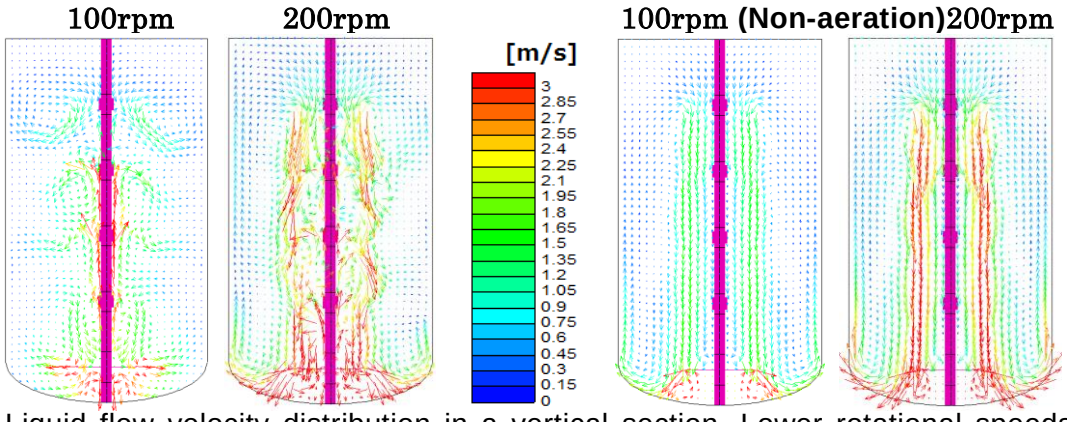
Liquid surface profile and liquid velocity distribution obtained by the VOF method (left) and spatial distribution of the Sauter mean diameter of the droplet (right).

Gas Absorption Simulation in Bioreactor

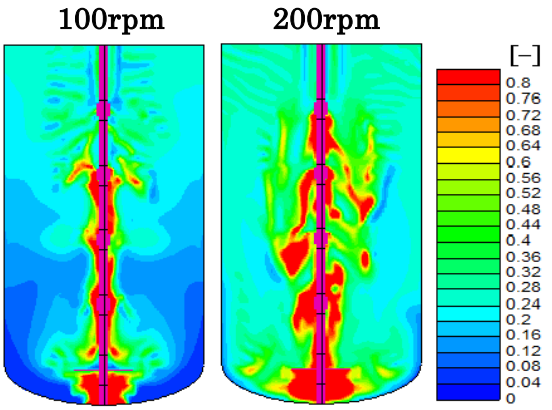
CFD simulation of an aerated bioreactor for cultivating micro-organisms such as animal cells. The oxygen component in the bubbles sparged by aeration is dissolved into the liquid as dissolved oxygen (DO) by gas absorption. In the liquid, DO is consumed by respiration of micro-organisms and carbon dioxide is released at the same time. In addition to kL_a, which is determined from the flow field, bubble void fraction and bubble diameter, dissolved oxygen, carbon dioxide, oxygen in bubbles, carbon dioxide and culture medium concentration in the liquid are also simulated with the liquid and gas flows. The bubble diameter distribution is also simulated using an N+1 (N dispersed phases and the continuous phase) multiphase fluid model considering the breakup and coalescence of bubbles.



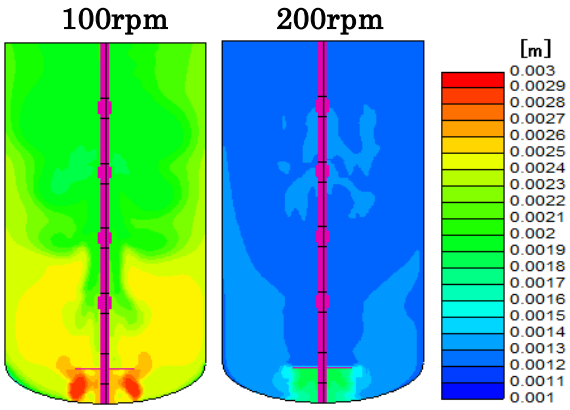
Main simulation conditions	
Tank Diameter	2[m]
Liquid depth	3.6[m]
Blade rotation speed	100/200[rpm]
Liquid density	1000[kg/m^3]
Liquid viscosity	0.001[Pas]
DO diffusion coefficient	3.3×10^{-9}[m^2/s]
DCO_2 diffusion coefficient	2.2×10^{-9}[m^2/s]
Sparged gas	air
Air flowrate	0.2[m^3/s]
Microbial respiration rate	0.0012[kg/m^{3}s]
Culture fluid injection vol.	0.001[m^3/s]



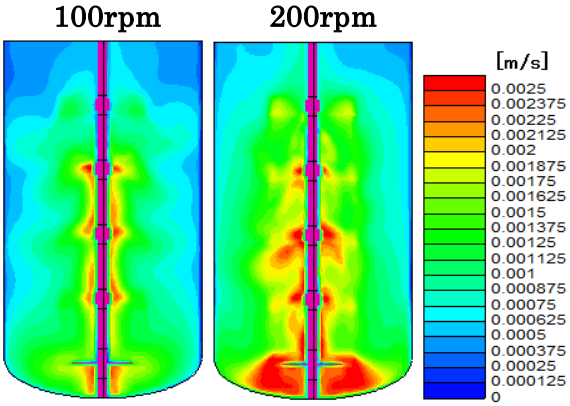
Liquid flow velocity distribution in a vertical section. Lower rotational speeds are more affected by aeration, which weakens the downward flow near the center. The figures on the right correspond to the cases without aeration (for reference).



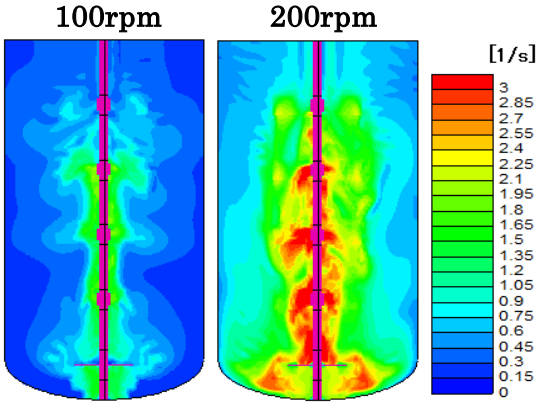
Spatial distributions of the bubble void fraction. The average of void fraction is 0.164 at 100 rpm and 0.265 at 200 rpm, with the mean value being greater at 200 rpm.



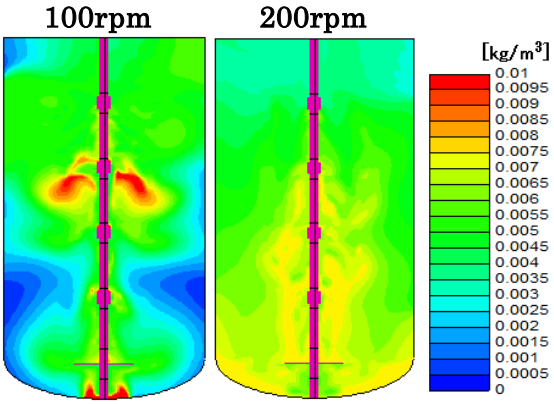
Spatial distributions of Sauter mean bubble diameter. The average of bubble diameter is 2.26 [mm] at 100 rpm and 1.20 [mm] at 200 rpm, with the bubble diameter being smaller at 200 rpm.



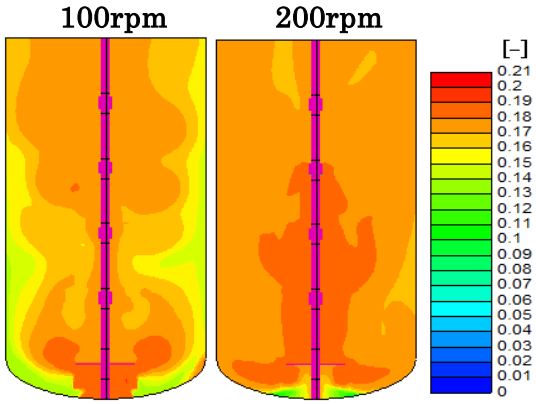
Spatial distributions of Oxygen k_L. The average of k_L is 0.000683 [m/s] at 100 rpm and 0.000968 [m/s] at 200 rpm, with the mean value being slightly higher at 200 rpm.



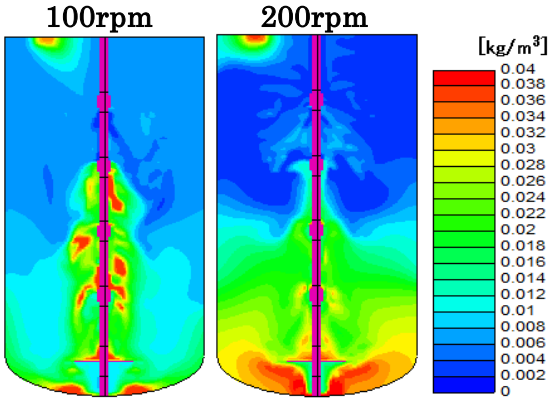
Spatial distributions of k_La (oxygen). The average of k_La is 0.252 [1/s] at 100 rpm and 0.944 [1/s] at 200 rpm, with the mean value being significantly larger at 200 rpm.



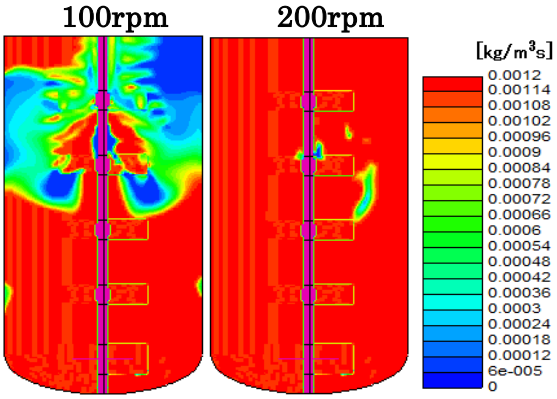
Spatial distributions of dissolved oxygen (DO) concentration in the liquid. The average is 0.00348 [kg/m3] at 100 rpm and 0.00548 [kg/m3] at 200 rpm.



Spatial distributions of Oxygen concentration in bubbles. The average is 0.170 at 100 rpm and 0.183 at 200 rpm.



Spatial distributions of culture medium concentration. The average value is 0.0121 [kg/m3] at 100 rpm and 0.0081 [kg/m3] at 200 rpm.



Spatial distributions of respiratory rate. At 100 rpm, there is a region in the upper part of the tank where sufficient respiration cannot be performed due to poor mixing.