Population balance modeling -an application in particle technology

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Link to Matlab:

www.glue.umd.edu/~sehrman/popbal.htm

Outline

- Aerosol reactors in industry
- Design problem, sneak peak
- Particle collection using cyclones
- Aerosol topics
  - size distributions
  - aggregates and fractals
  - coagulation/breakup
- Population balance equations
- Discrete and sectional approach
- Design problem, revisited

Acknowledgments

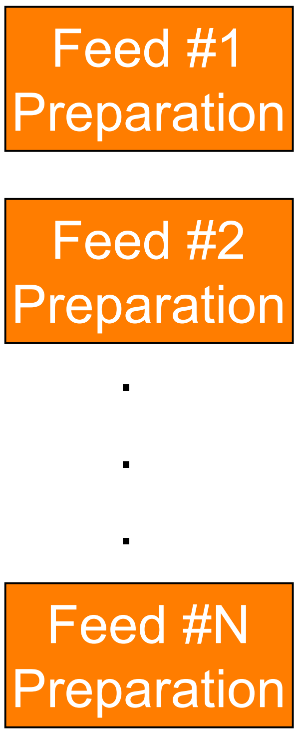
- Population balance lectures and design problems developed in collaboration with Dr. R. Bertrum Diemer, Principal Consultant, Chemical Reaction Engineering, DuPont, Wilmington DE, USA
- Matlab code: Brendan Hoffman, Kelly Tipton, Yechun Wang, Matt McHale, Spring 2003 students
- Support from US National Science Foundation & DuPont

- Purpose
  - increase interest in field of particle technology
  - show practical application of population balance modeling approach

Important aerosol products

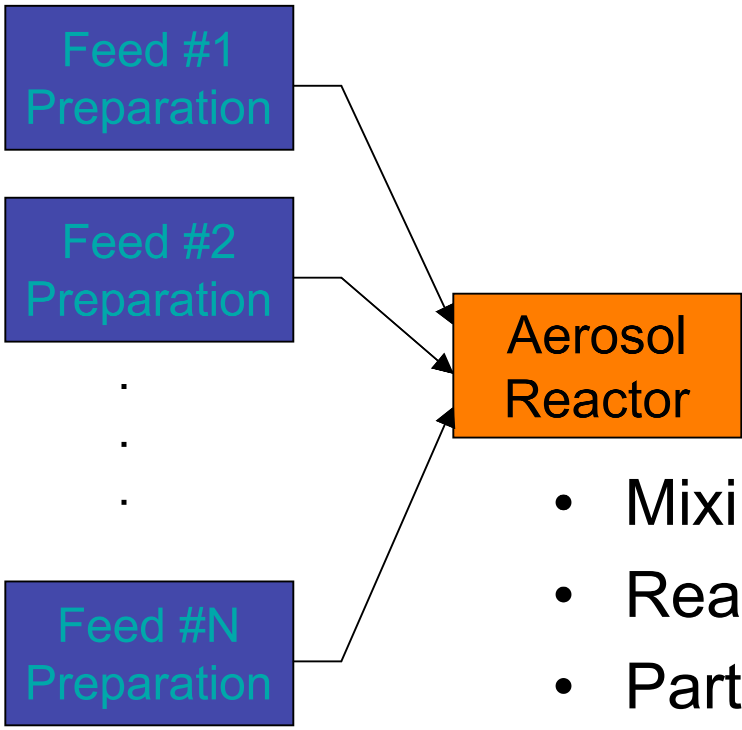
- Silica
- Titania
- Carbon black
- Specialty materials
  - Nano zinc oxide used today in sunscreen
  - High surface area catalyst supports (alumina, zirconia, etc..)
  - Chemical mechanical polishing agents (ceria, silica, etc…)

General Aerosol Process Schematic



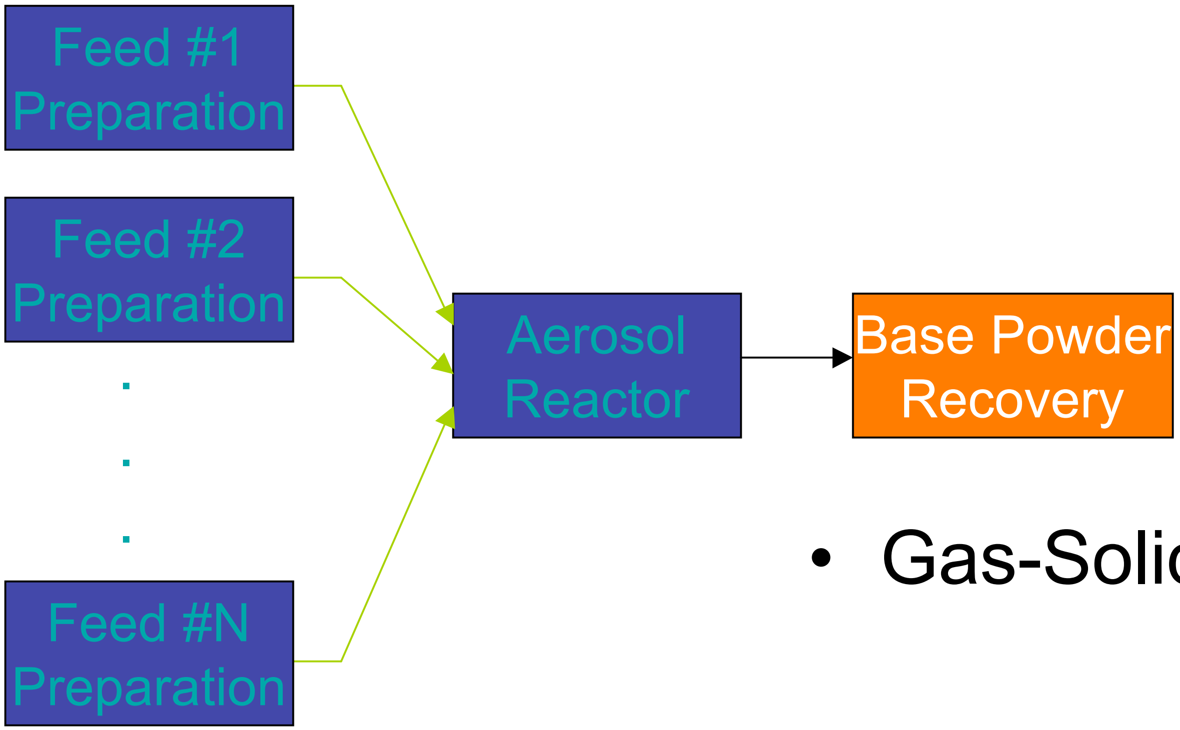
- Vaporization
- Pumping/Compression
- Addition of additives
- Preheating

General Aerosol Process Schematic



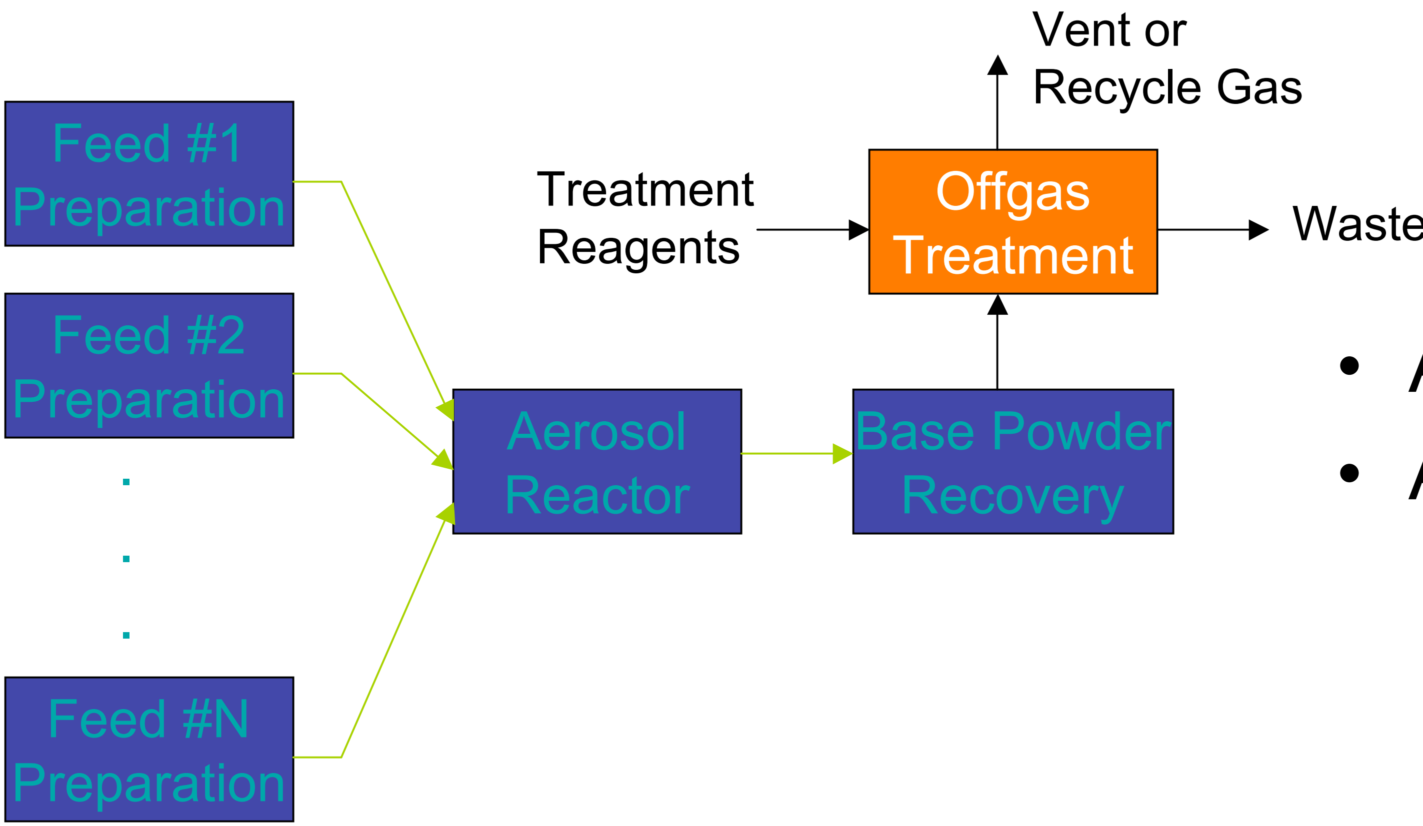
- Mixing
- Reaction Residence Time
- Particle Formation/Growth Control
- Agglomeration Control
- Cooling/Heating
- Wall Scale Removal

General Aerosol Process Schematic



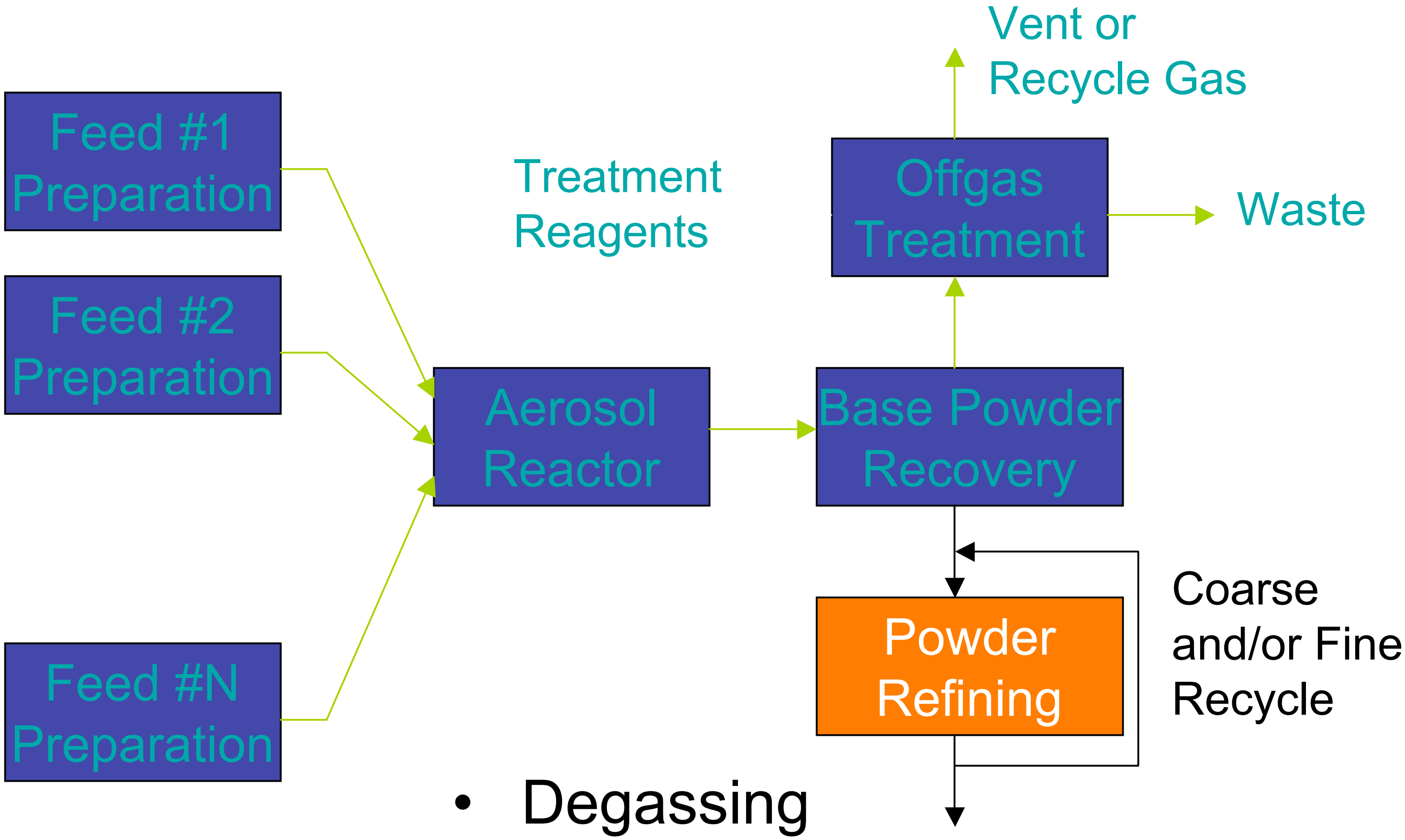
- Gas-Solid Separation

General Aerosol Process Schematic



- Absorption
- Adsorption

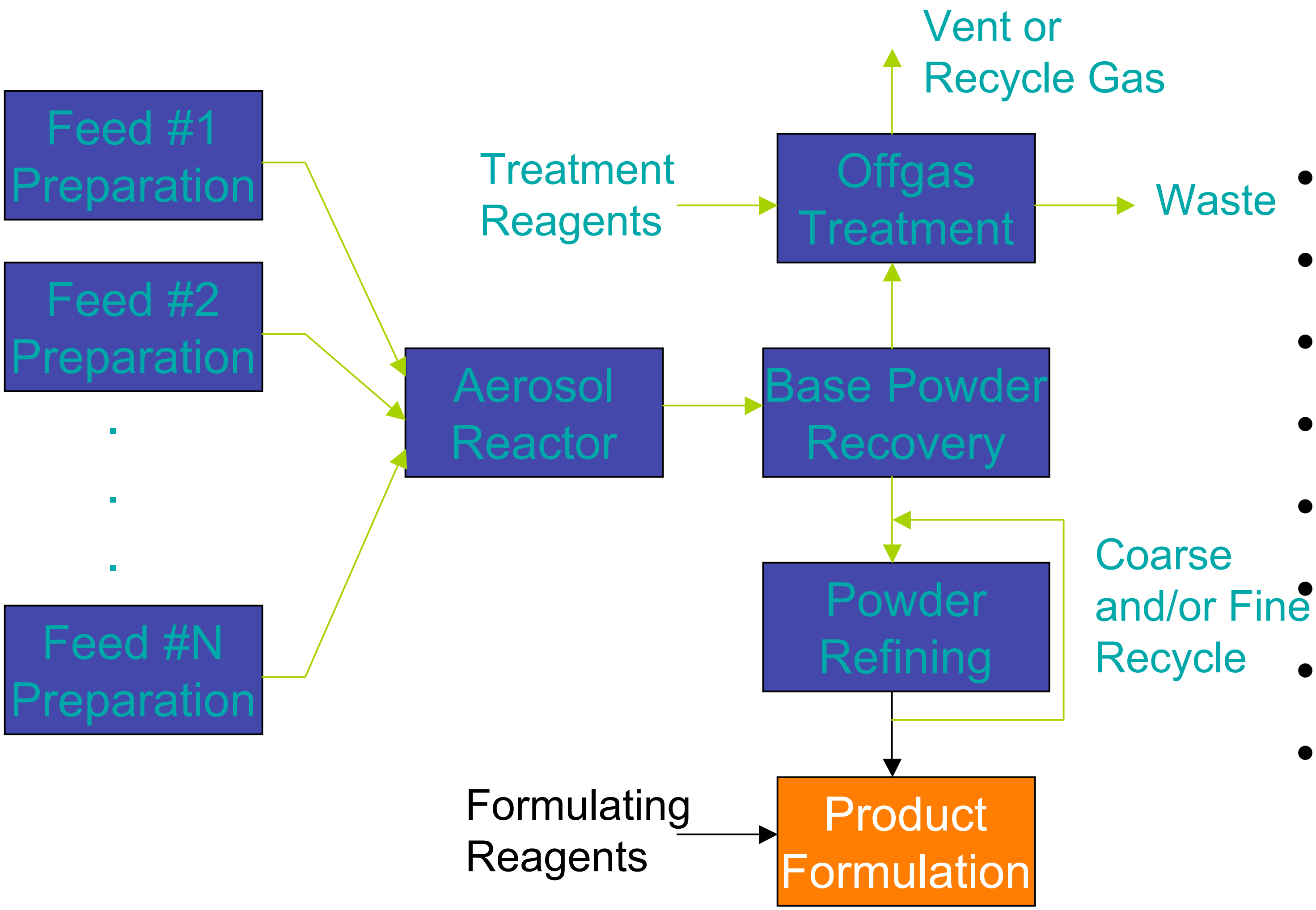
General Aerosol Process Schematic



- Degassing
- Desorption
- Conveying

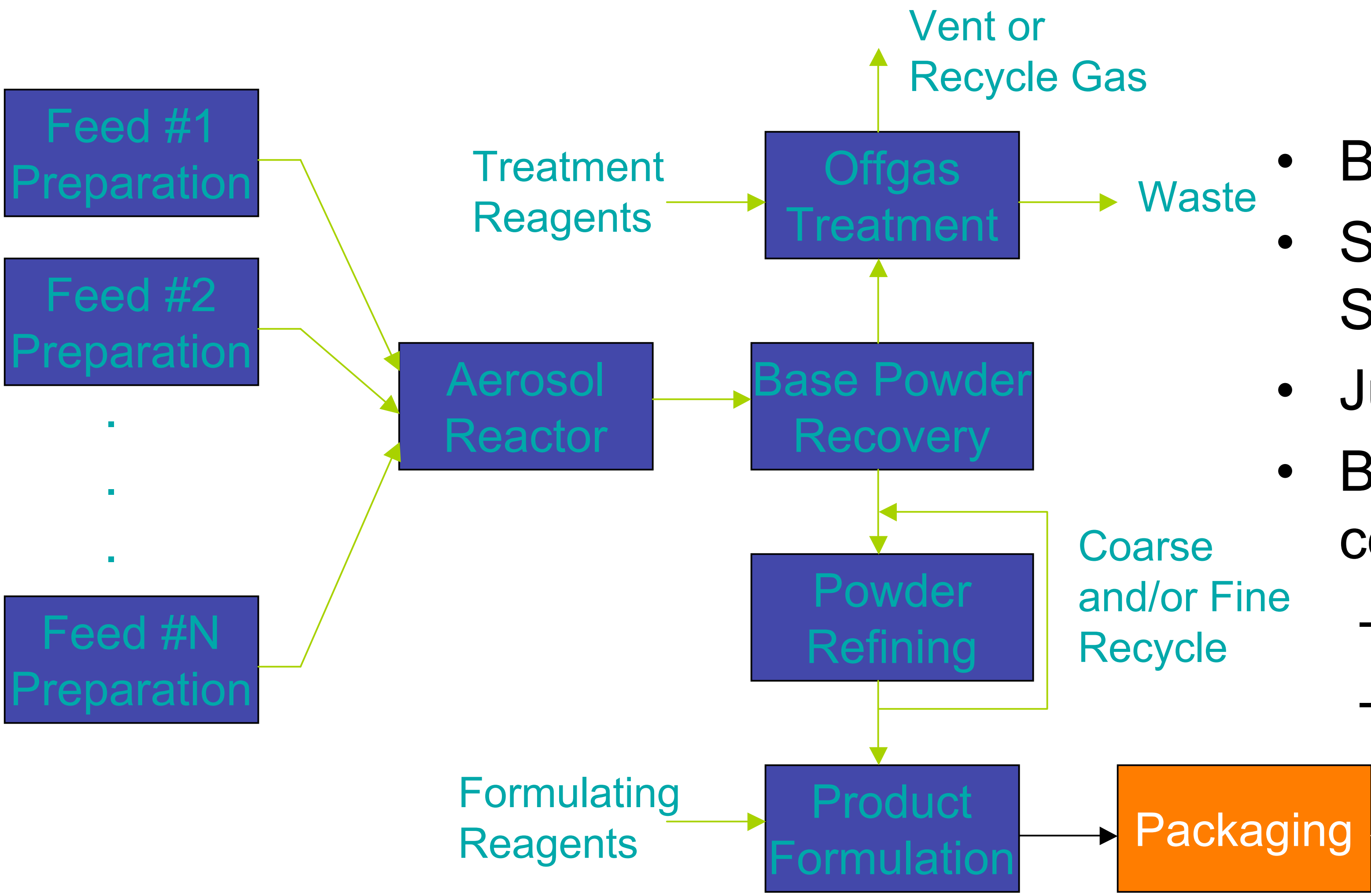
- Size Modification
- Solid Separations

General Aerosol Process Schematic



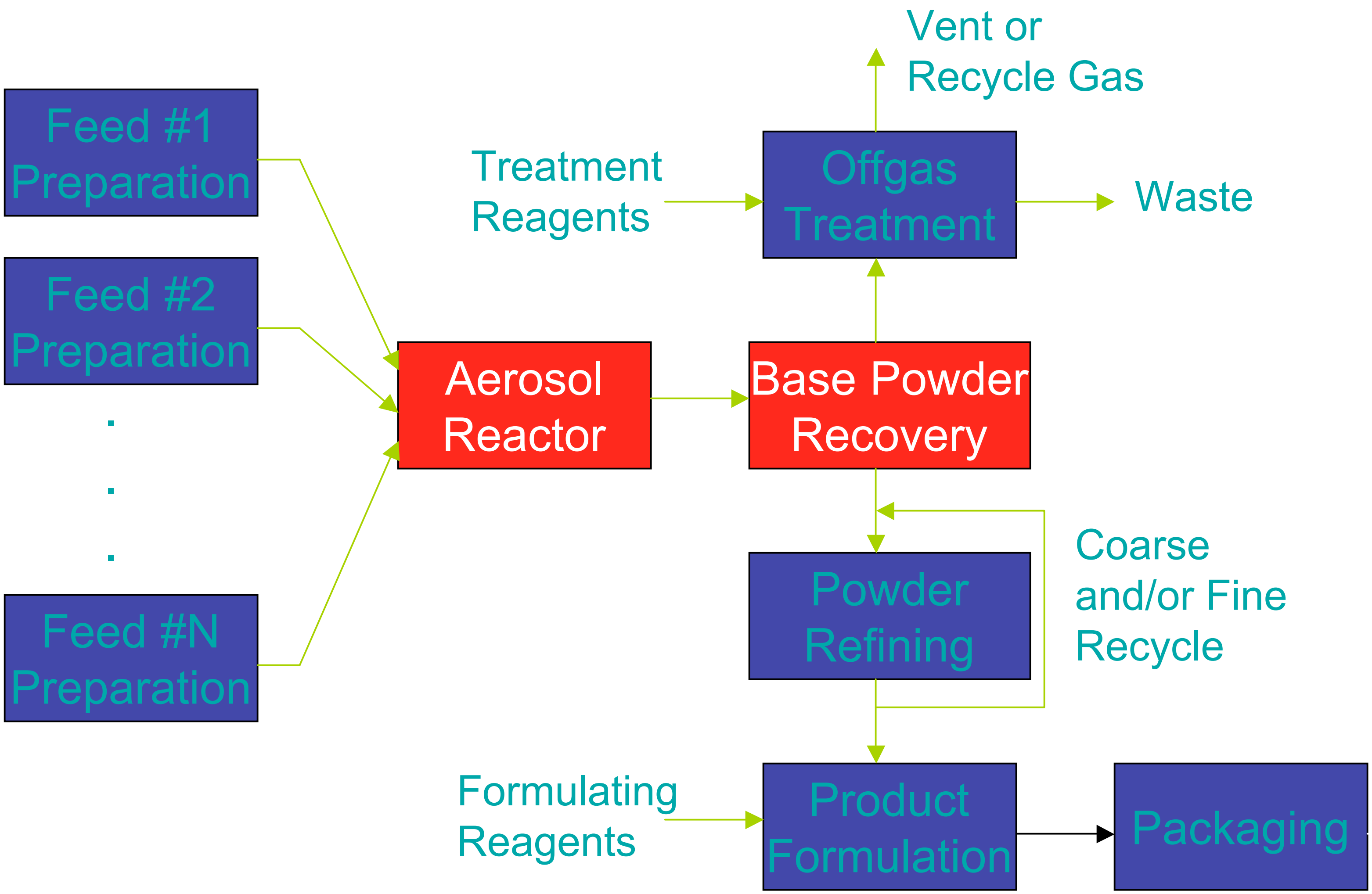
- Coating
- Additives
- Tabletting
- Briquetting
- Granulation
- Slurrying
- Filtration
- Drying

General Aerosol Process Schematic



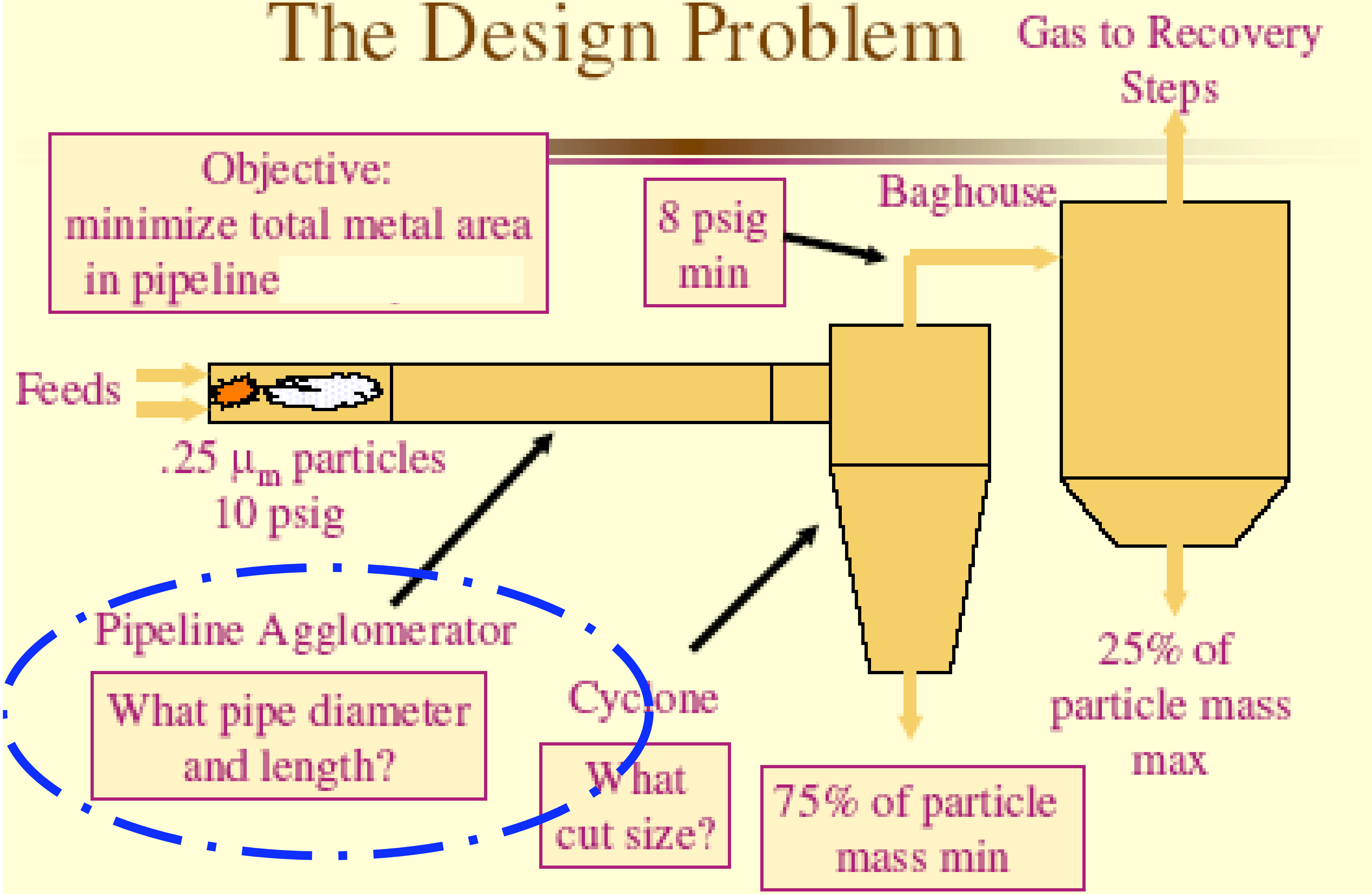
- Bags
- Super Sacks
- Jugs
- Bulk containers
  - trucks
  - tank cars

General Aerosol Process Schematic

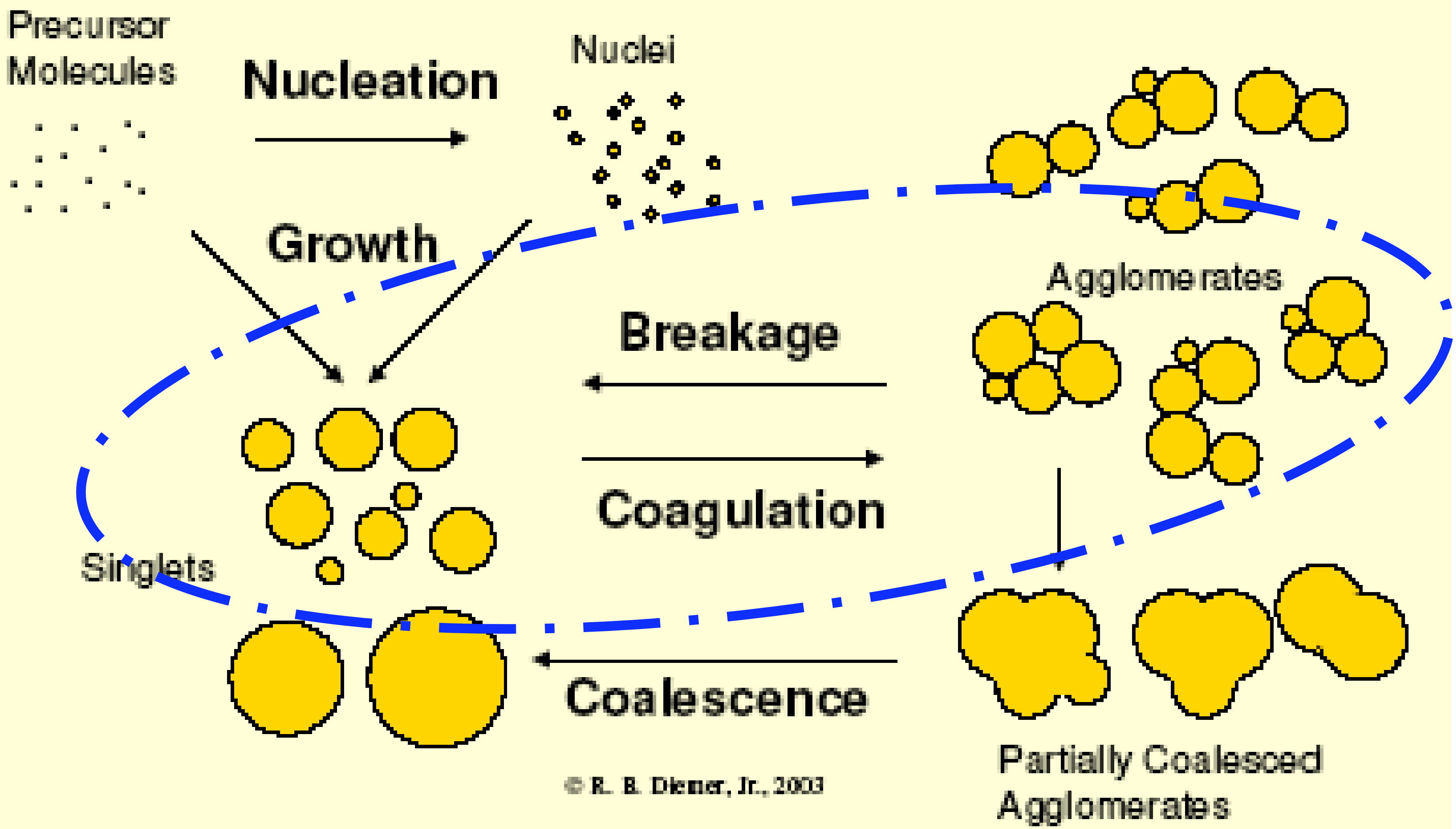


Our focus, reactor and gas solid separation

The Design Problem



Particle Formation, Growth & Transformation



Thermal Carbon Black Process

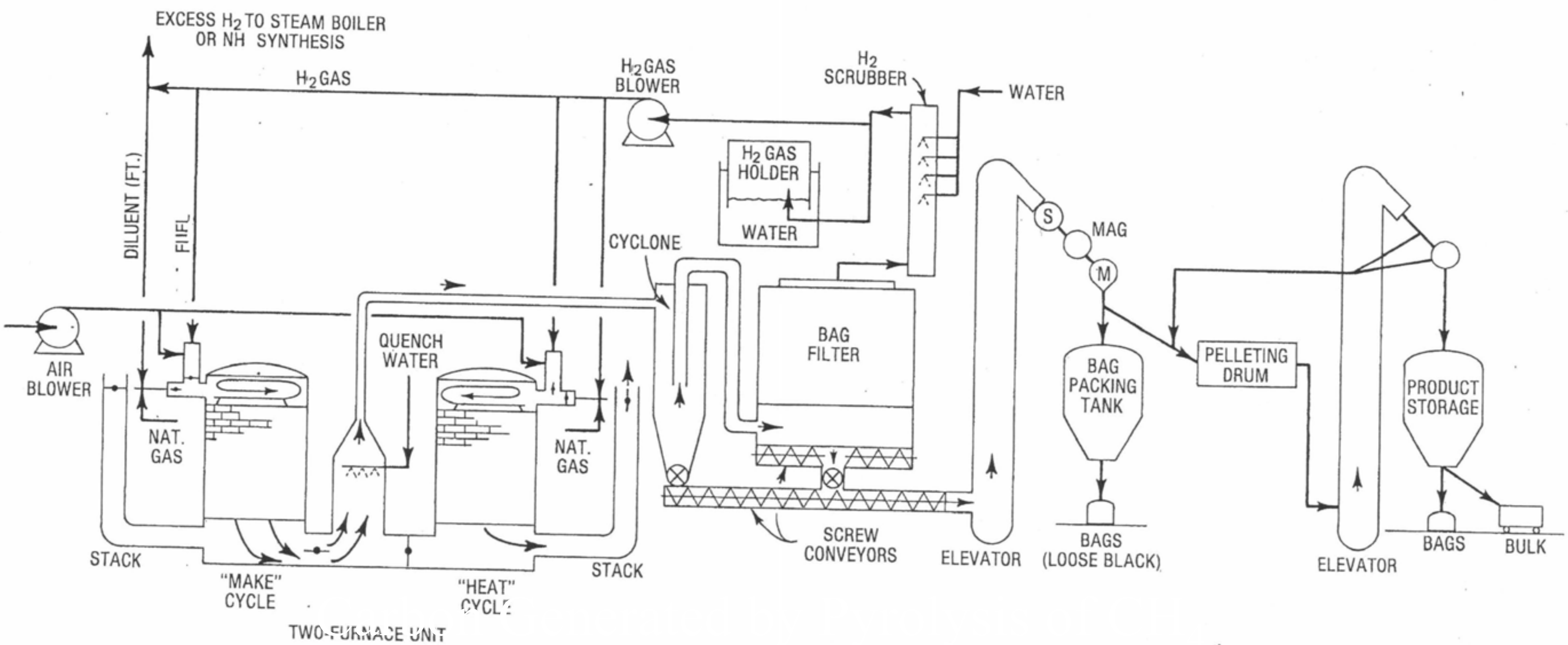


FIG. 26. Thermal process (natural gas feedstock).

Johnson, P. H., and Eberline, C. R., "Carbon Black, Furnace Black", *Encyclopedia of Chemical Processing and Design*, J. J. McKetta, ed., Vol. 6, Marcel Dekker, 1978, pp. 187-257.

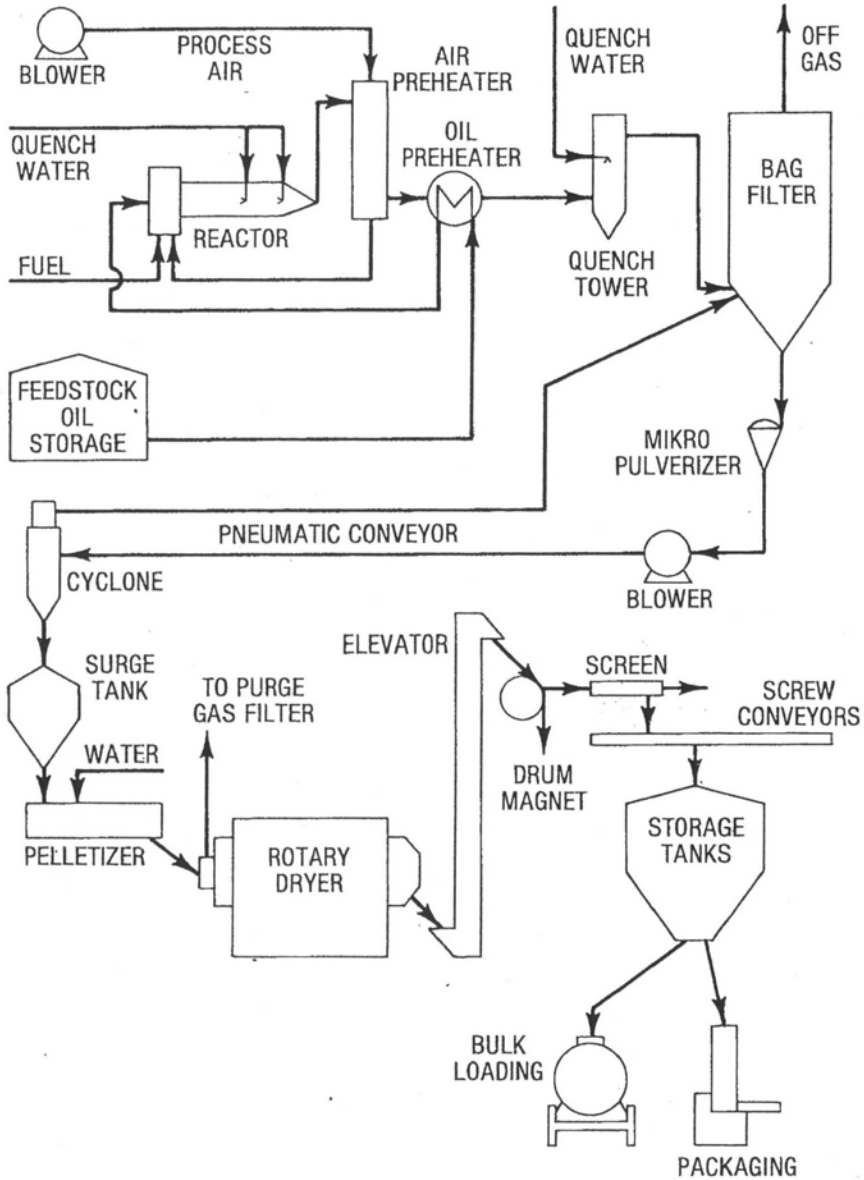


FIG. 18. Oil furnace carbon black process.

Furnace Carbon Black Process

Johnson, P. H., and Eberline, C. R., "Carbon Black, Furnace Black", *Encyclopedia of Chemical Processing and Design*, J. J. McKetta, ed., Vol. 6, Marcel Dekker, 1978, pp. 187-257.

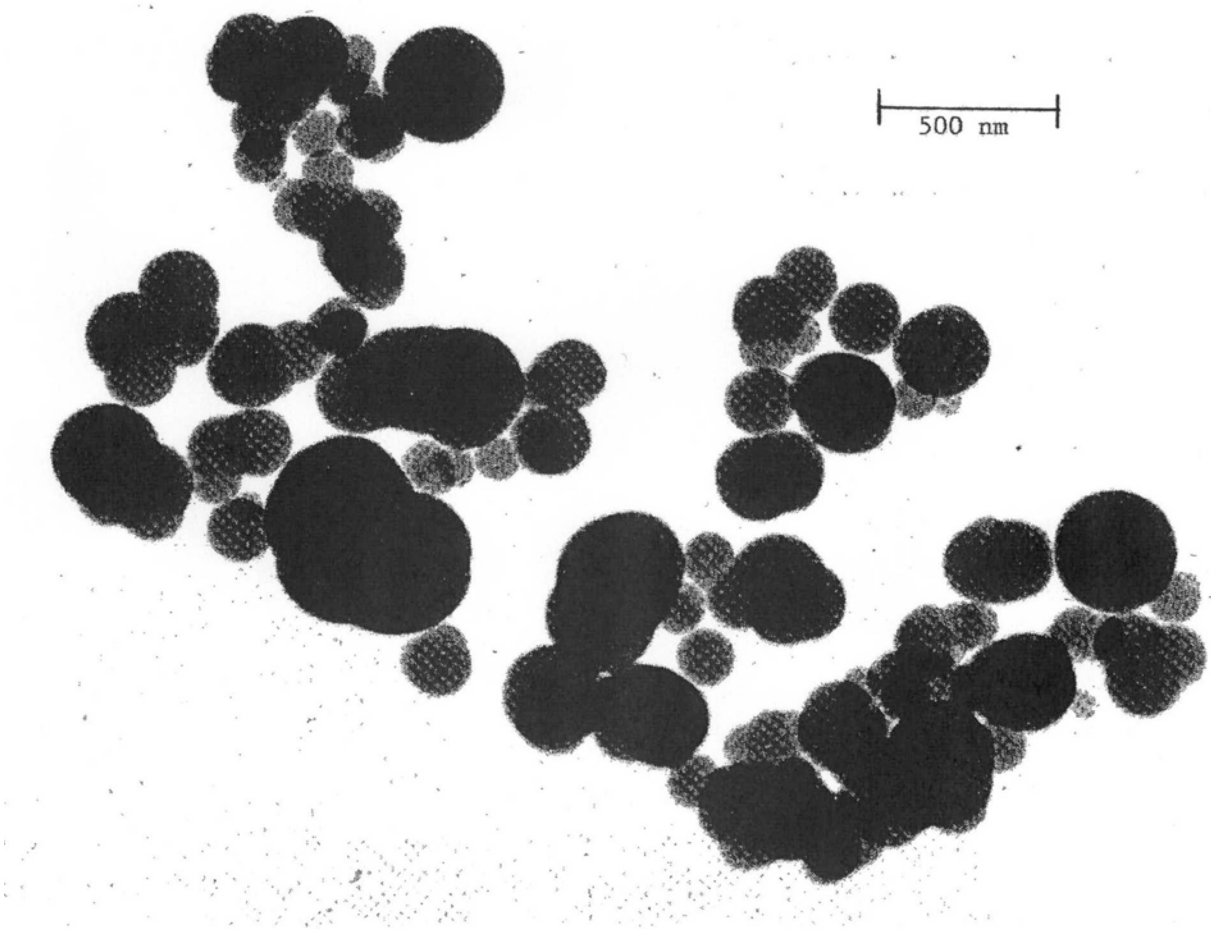


FIG. 7. Thermal black.

Thermal Carbon Black

- ~200 nm Primary Particles
- 4-6 Primaries/ Agglomerate

Johnson, P. H., and Eberline, C. R., “Carbon Black, Furnace Black”, *Encyclopedia of Chemical Processing and Design*, J. J. McKetta, ed., Vol. 6, Marcel Dekker, 1978, pp. 187-257.

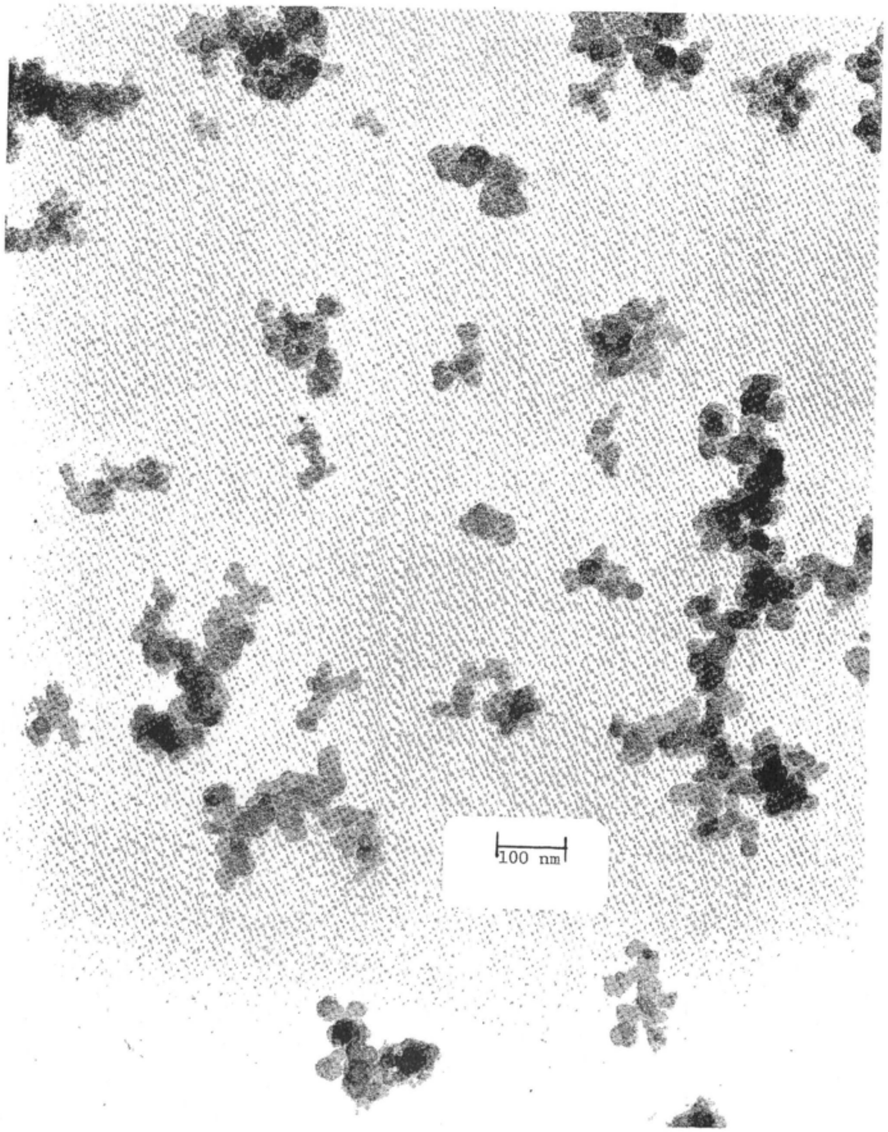


FIG. 8. A structured oil-furnace black.

Oil-Furnace Carbon Black

- ~20 nm Primary Particles
- 10-50 Primaries/ Agglomerate

Johnson, P. H., and Eberline, C. R., “Carbon Black, Furnace Black”, *Encyclopedia of Chemical Processing and Design*, J. J. McKetta, ed., Vol. 6, Marcel Dekker, 1978, pp. 187-257.

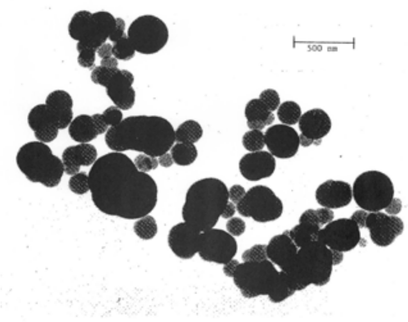


FIG. 7. Thermal black.

What do you see?

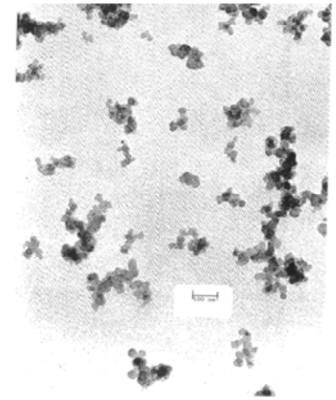


FIG. 8. A structured oil-furnace black.

- What do you notice about each sample?

- How do the two images differ?

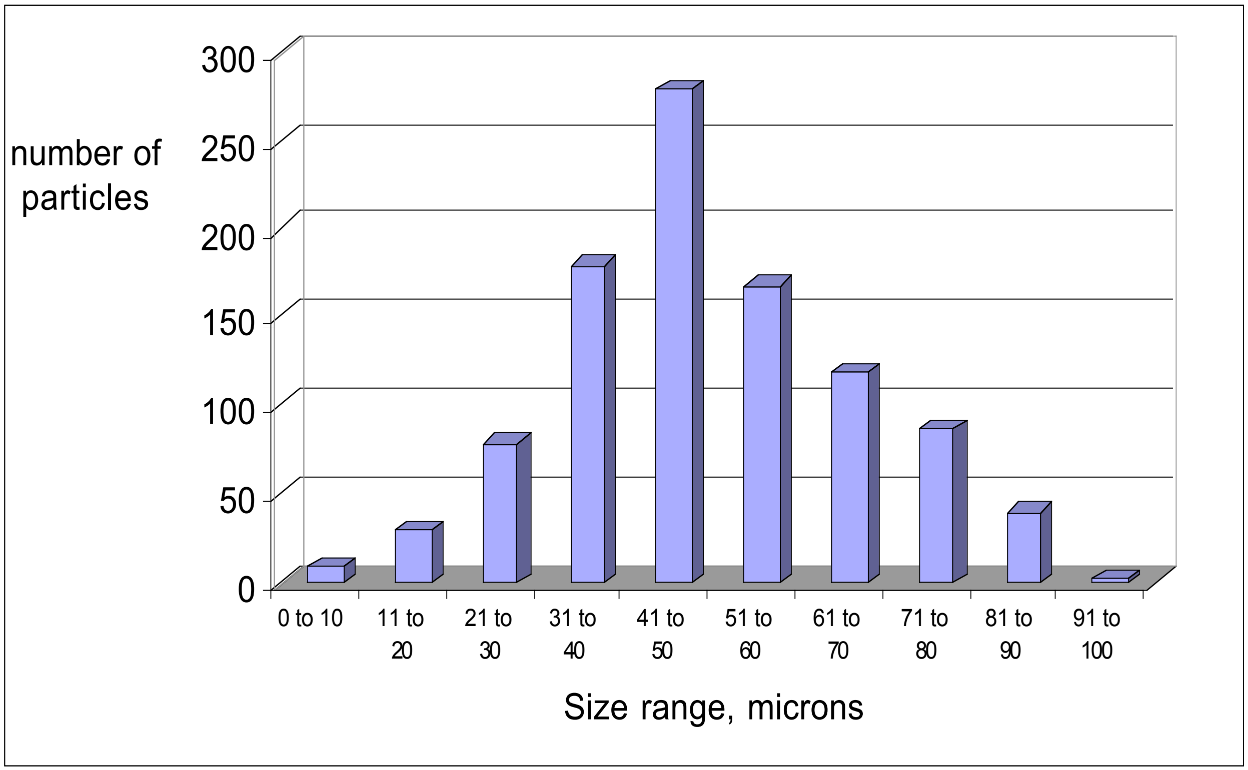
Particles not all same…

- Diameter
- Volume
- Surface area
- Structure

How to represent size distributions, histogram example:

Size range, microns	number of particles
0 to 10	10
11 to 20	30
21 to 30	80
31 to 40	180
41 to 50	280
51 to 60	169
61 to 70	120
71 to 80	88
81 to 90	40
91 to 100	3

Number of particles vs particle diameter

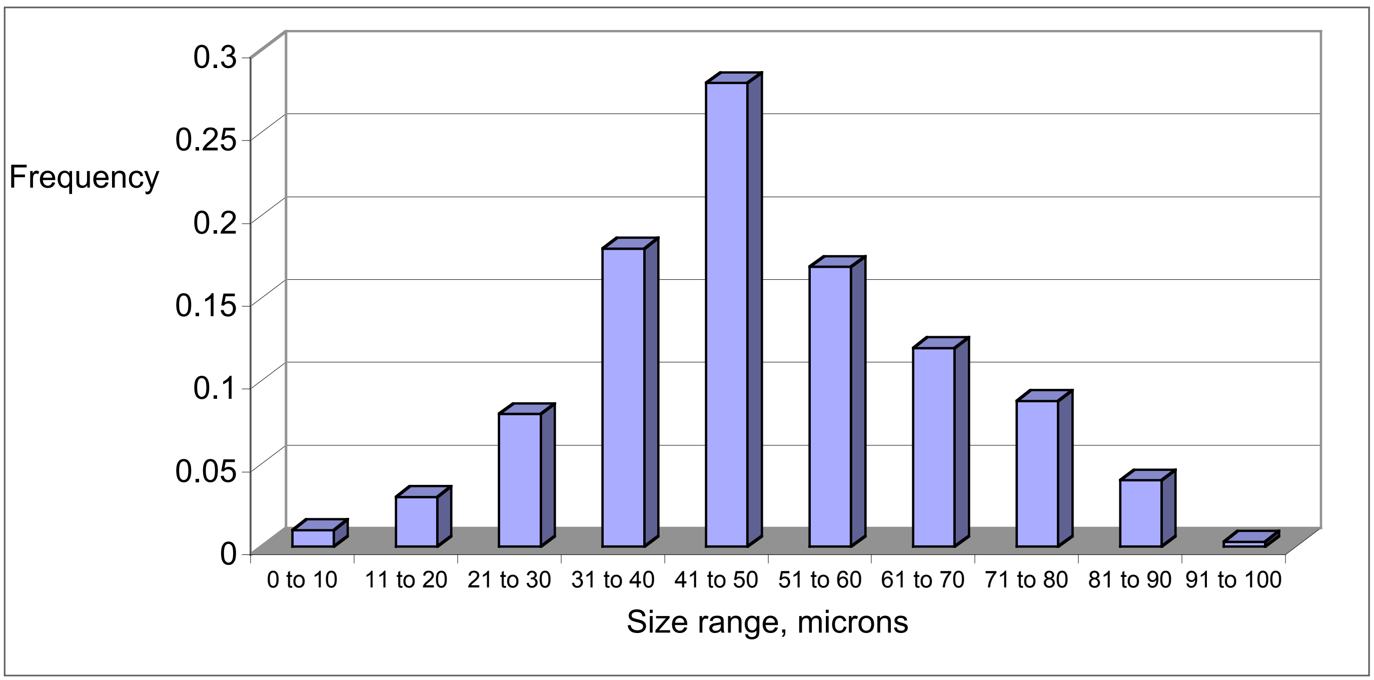


Can create histogram from raw particle size data using Analysis tool pack add-in, with Excel.. After add-in, go to ‘tools’, then ‘data analysis’, then ‘histogram’.

How to represent size distributions, histogram example:

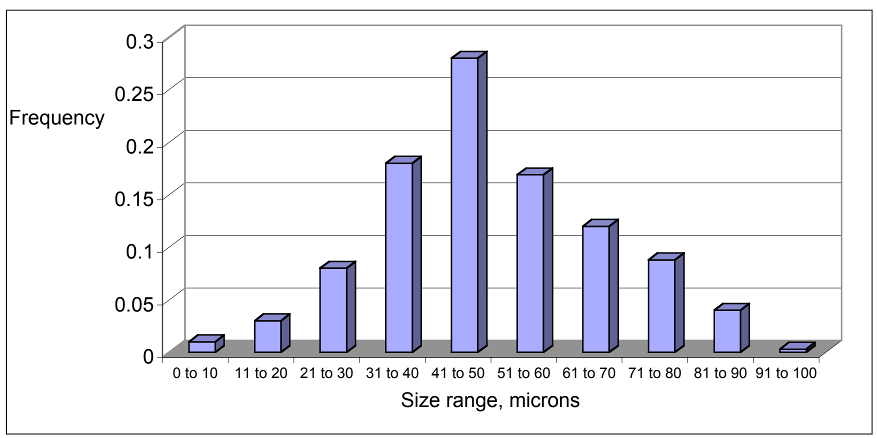
Size range, microns	number of pa	Frequency
0 to 10	10	0.01
11 to 20	30	0.03
21 to 30	80	0.08
31 to 40	180	0.18
41 to 50	280	0.28
51 to 60	169	0.169
61 to 70	120	0.12
71 to 80	88	0.088
81 to 90	40	0.04
91 to 100	3	0.003
total number	1000	

Number frequency vs particle diameter



Test yourself…

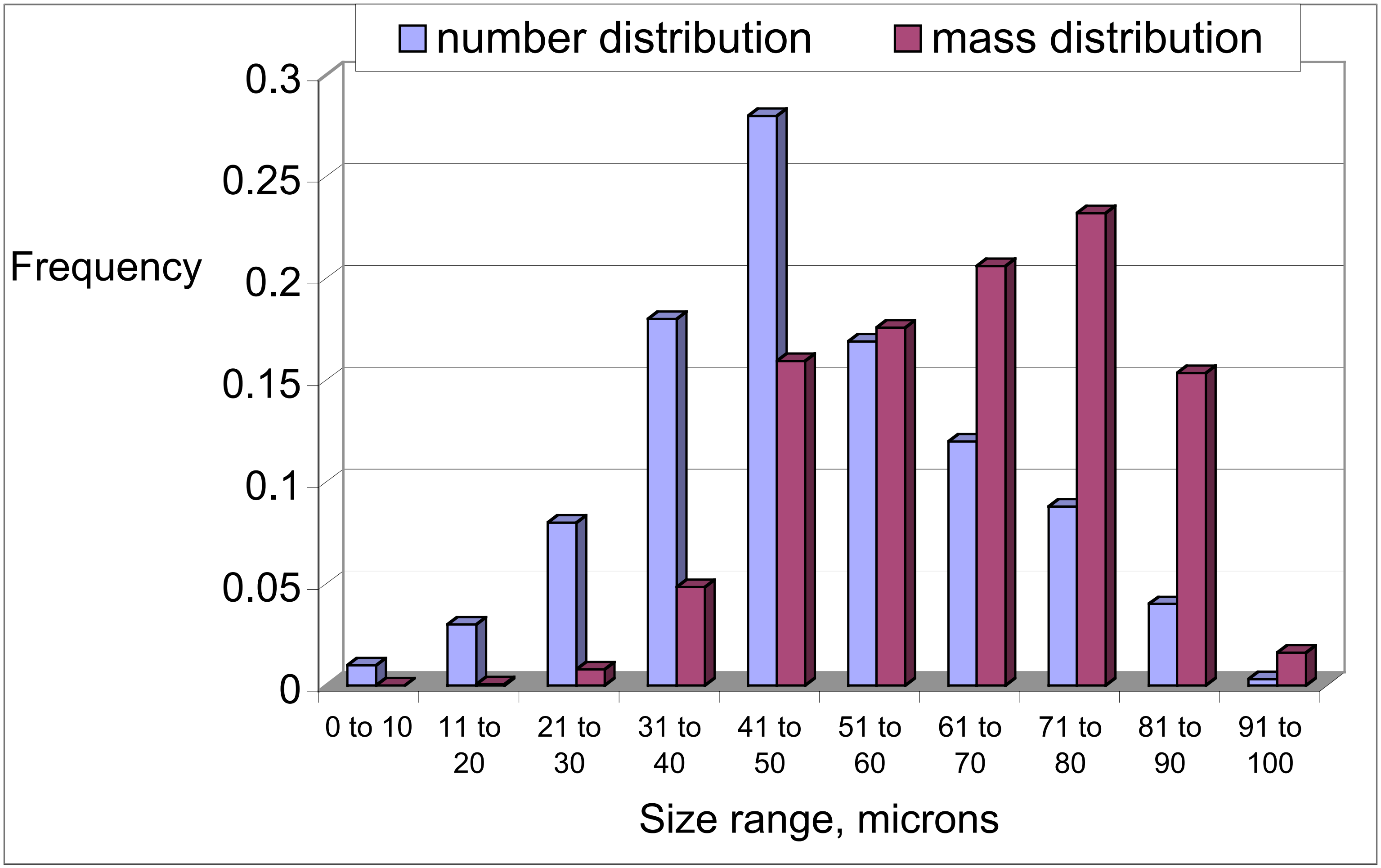
- If you change the frequency distribution so that is based on the MASS of particles in each size range versus the NUMBER, will the shape of the frequency distribution change?



More spreadsheet manipulations

Size range, microns	number of particles	Frequency	assume diameter	mass of particles in each bin, g	Mass frequency
0 to 10	10	0.01	5	6.54E-10	0.00
11 to 20	30	0.03	15	5.30E-08	0.00
21 to 30	80	0.08	25	6.54E-07	0.01
31 to 40	180	0.18	35	4.04E-06	0.05
41 to 50	280	0.28	45	1.34E-05	0.16
51 to 60	169	0.169	55	1.47E-05	0.18
61 to 70	120	0.12	65	1.72E-05	0.21
71 to 80	88	0.088	75	1.94E-05	0.23
81 to 90	40	0.04	85	1.29E-05	0.15
91 to 100	3	0.003	95	1.35E-06	0.02
total number	1000				
total mass assuming 1g/cc density				8.37E-05	

Number vs mass distribution



Continuous distributions

Also useful: continuous distributions, where some function, n_d, describes the number of particles of some diameter d_p at a given point, at a given time.

In terms of number concentration:

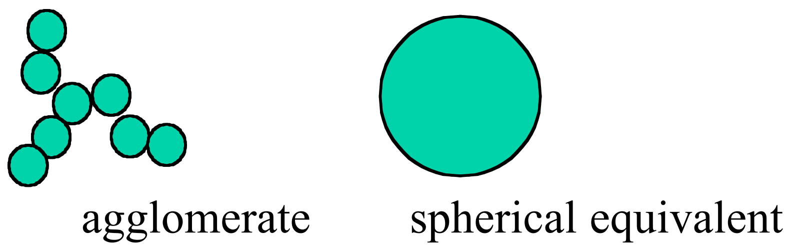
Let dN = number of particles per unit volume of gas at a given position in space (represented by position vector **r**), at a given time (t), in the particle range d_p to $d_p + d(d_p)$. N = total number of particles per unit volume of gas at a given position in space at a given time. Size distribution function is defined as:

$$n_d(d_p, \mathbf{r}, t) = \frac{dN}{d(d_p)}$$

Can also have size distribution function, n, with particle volume v as size parameter: $n(v, \mathbf{r}, t) = \frac{dN}{dv}$

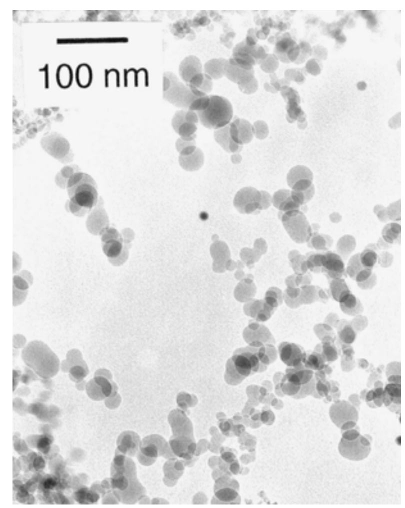
Aggregates of hard spheres

- When primary particles collide and stick, but do not coalesce, irregular structures are formed



how should these structures be characterized?

- Radius gives space taken up, but no information about mass/actual volume. Using only actual volume doesn't indicate how much space it takes up.
- Real flame generated aerosol:



Concept of fractal dimension

- Aerosol particles which consist of agglomerates of ‘primary particles’, (often, combustion generated) may be described using the concept of fractals.
- Fractals - The relationship between diameter of aerosol agglomerates, and the volume of primary particles in the agglomerate can be written:

$$\frac{v}{v_o} = \left(\frac{d}{d_0}\right)^{D_f} \quad \text{where } v_o = \frac{\pi}{6}\, d_0^3$$

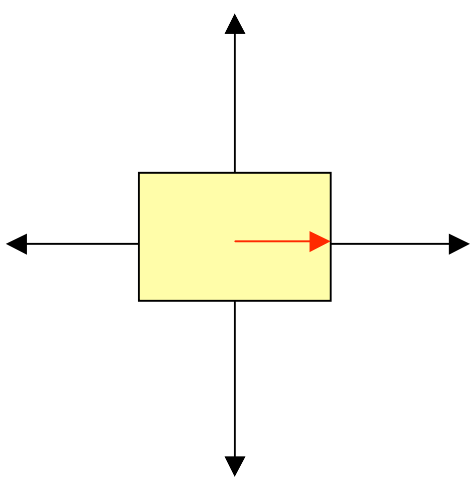
is the volume of the primary particle of diameter d_o

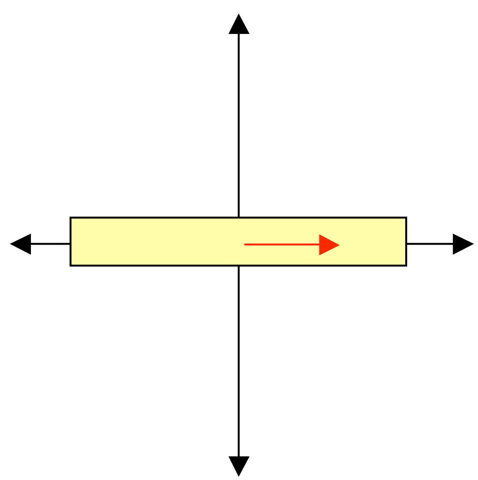
- d typically based on 2 * radius of gyration

Radius of Gyration

"The Radius of Gyration of an Area about a given axis is a distance k from the axis. At this distance k an equivalent area is thought of as a **Line Area** parallel to the original axis. The moment of inertia of this **Line Area** about the original axis is unchanged."

http://www.efunda.com/math/areas/RadiusOfGyrationDef.cfm

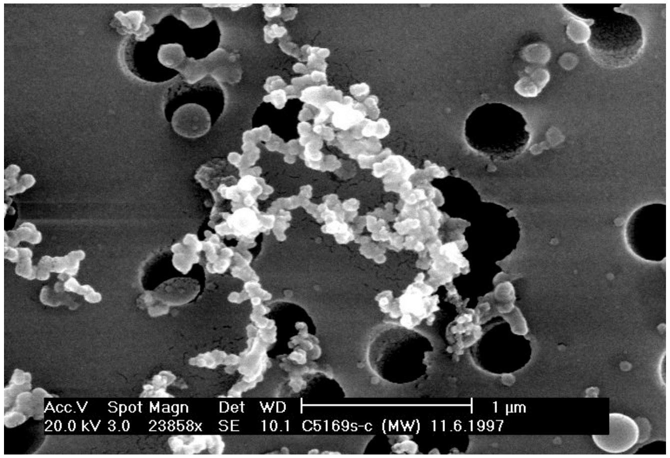




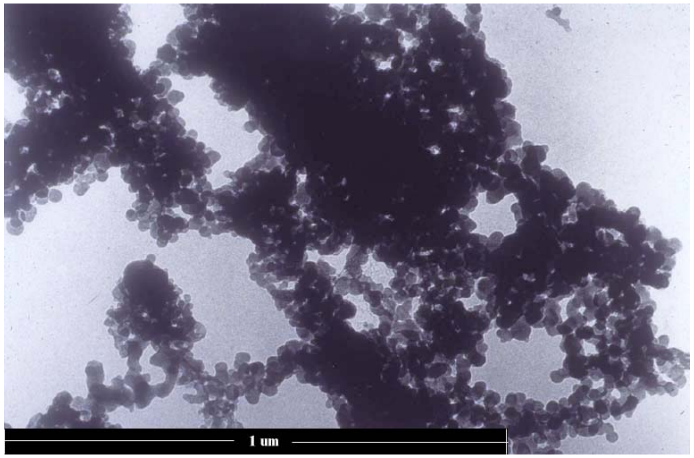
Fractal dimension

- Fractals - D_f = 2 = uniform density in a plane, D_f of 3 = uniform density in three dimensions
- Typical values for agglomerates ranges from 1.5 to near 3 depending on mechanism of agglomeration, possible rearrangement, and external field effects
- Small agglomerates (few particles) not really fractal but "fractal-like"
- For hundreds of particles, relationship holds well

Test yourself…



http://www.mpch-mainz.mpg.de/~gth/soot1.jpg



http://faculty.engineering.ucdavis.edu/jenkins/previous/August2002/16_23.jpg

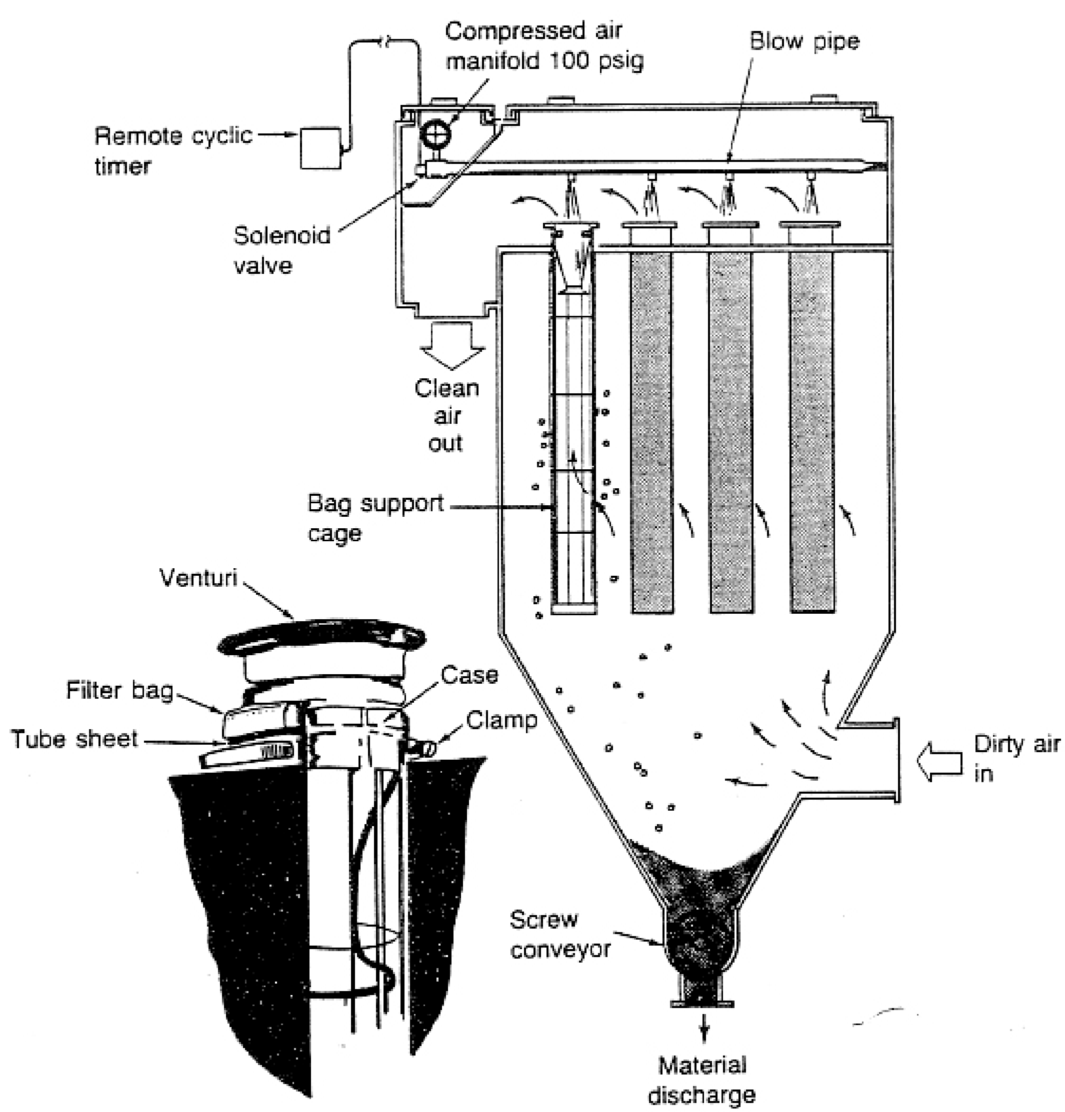
Which picture shows particle agglomerates with a lower fractal dimension?

Working backwards in the problem

- Particle gas separators
- Use different phenomena
  - Gravitational settlers
  - Filters (baghouse)
  - Scrubbers
  - Inertial separators (cyclone)
  - Electrostatic precipitators

Pulse Jet Baghouse

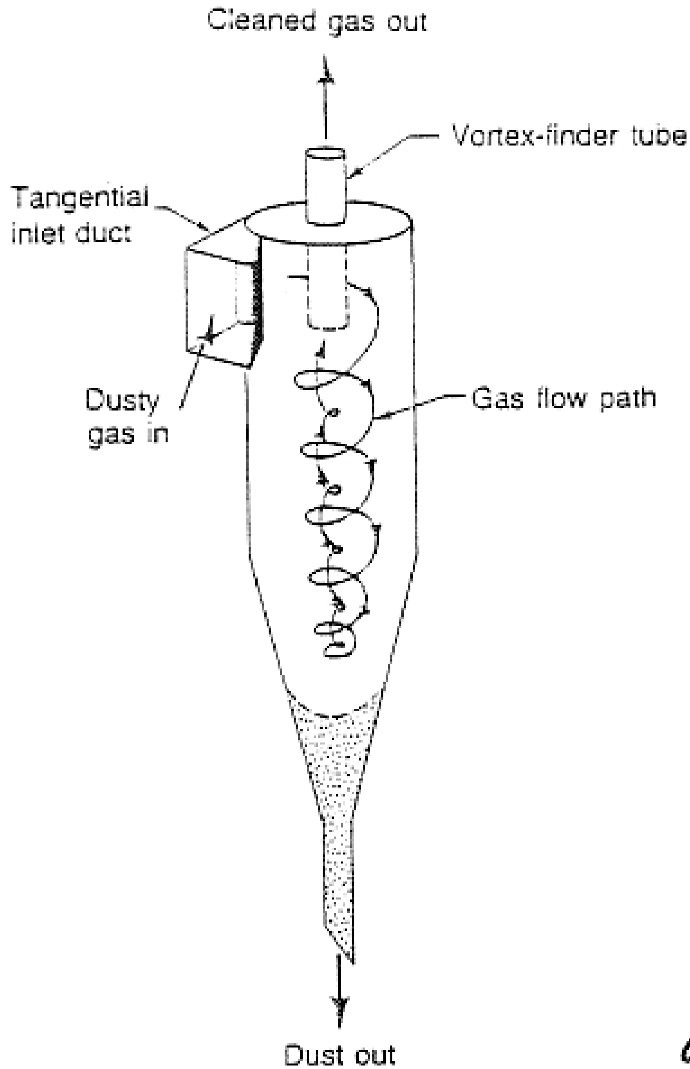
Figure 6.6 Schematic diagram of a pulse-jet baghouse.



Air Pollution Control: A Design Approach
Cooper & Alley, PWS Eng. Boston 1986

Standard Cyclone

Figure 4.1 Schematic flow diagram of a standard cyclone.



air Pollution control
cooper & Alley 1986

Force balance on particle in cyclone

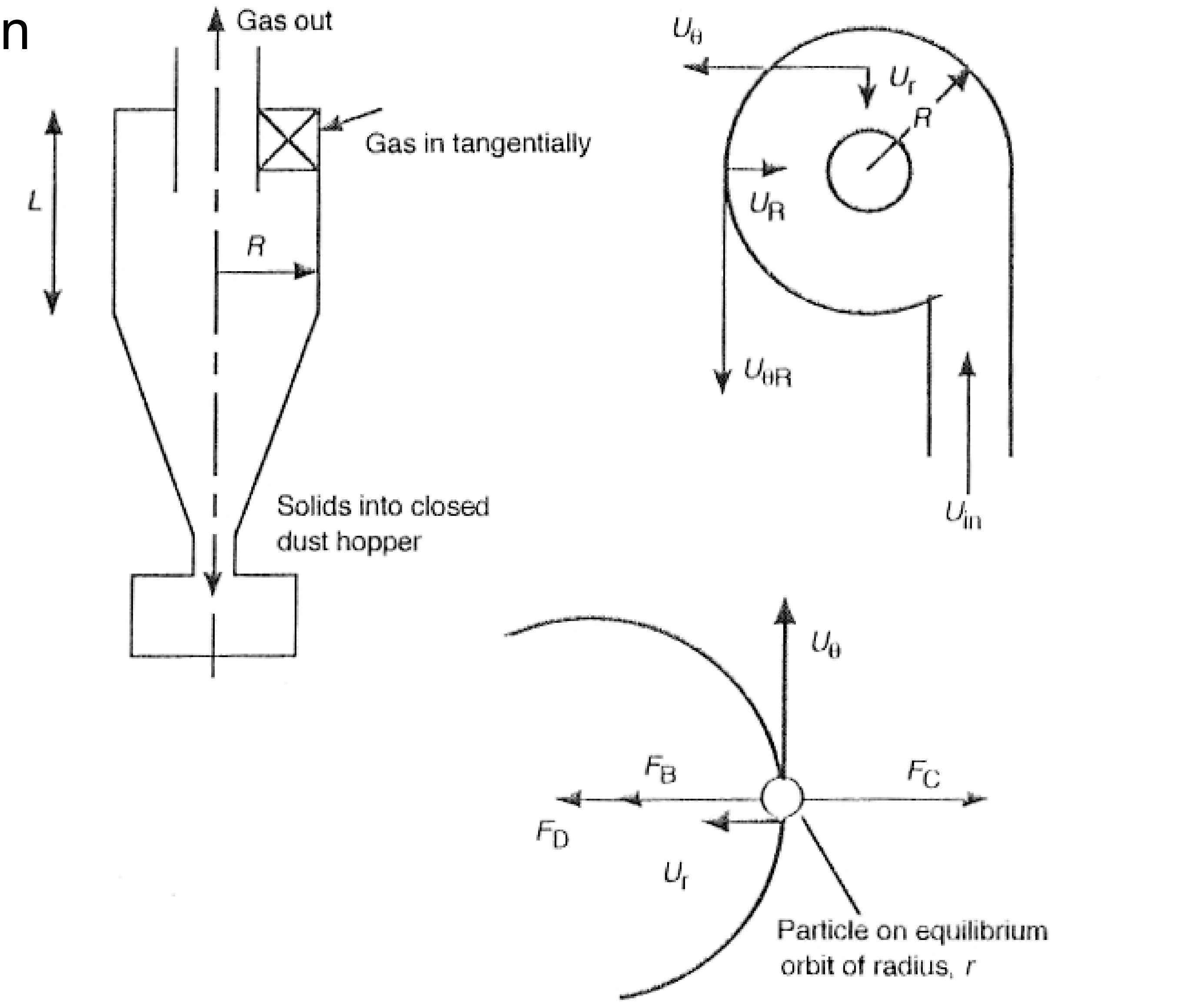
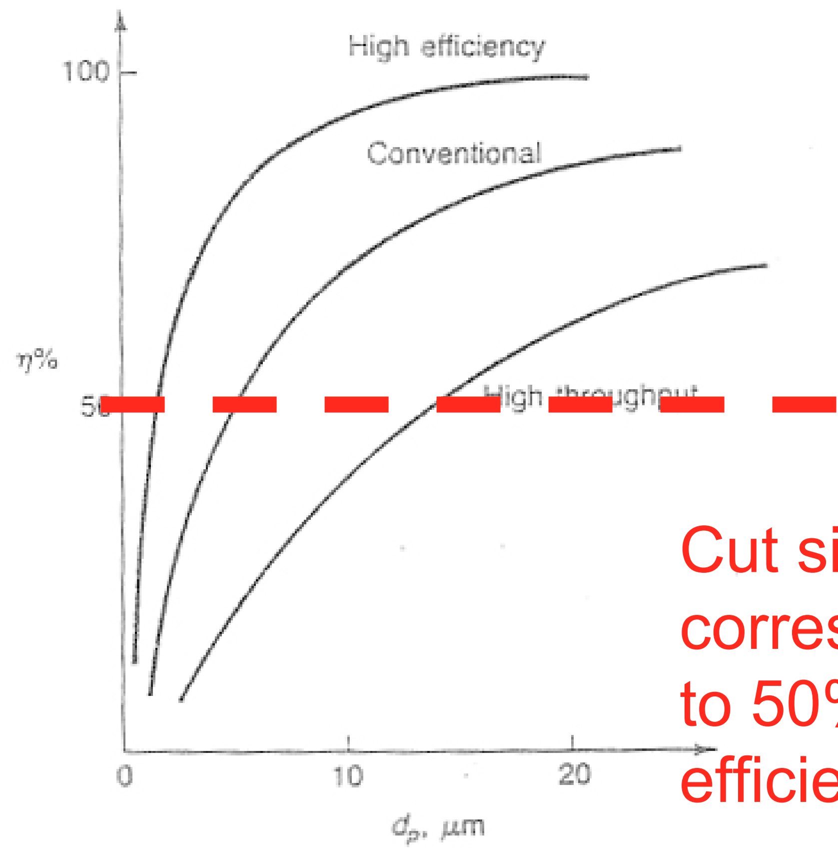


Figure 7.3 Reverse flow cyclone – a simple theory for separation efficiency

Rhodes, Introduction to Particle Technology, Wiley, 1998

Cyclone Efficiency as Function of Particle Diameter

Figure 4.3 General relationship of collection efficiency versus particle size for cyclones.



NOTE: Efficiency versus size curves represent broad generalizations, not exact relationships.

Cut size = diameter corresponding to 50% collection efficiency

Which type has lowest pressure drop?

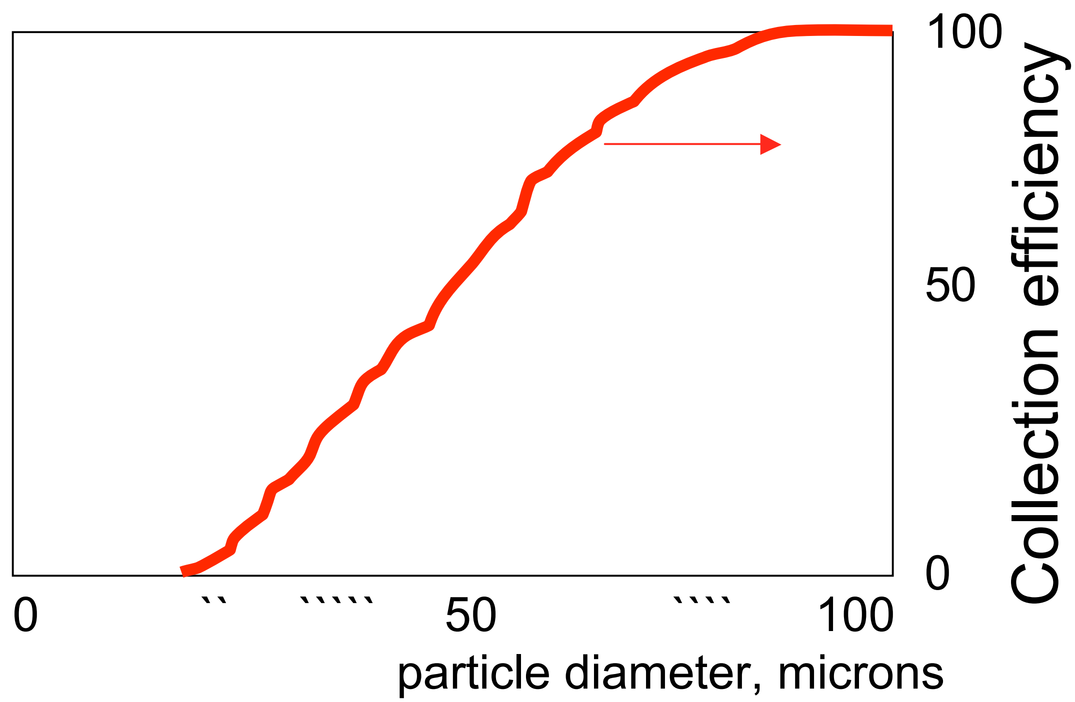
Air Pollution Control: A design approach
Cooper & Alley PWS Engineering, Boston 1986

Cyclones

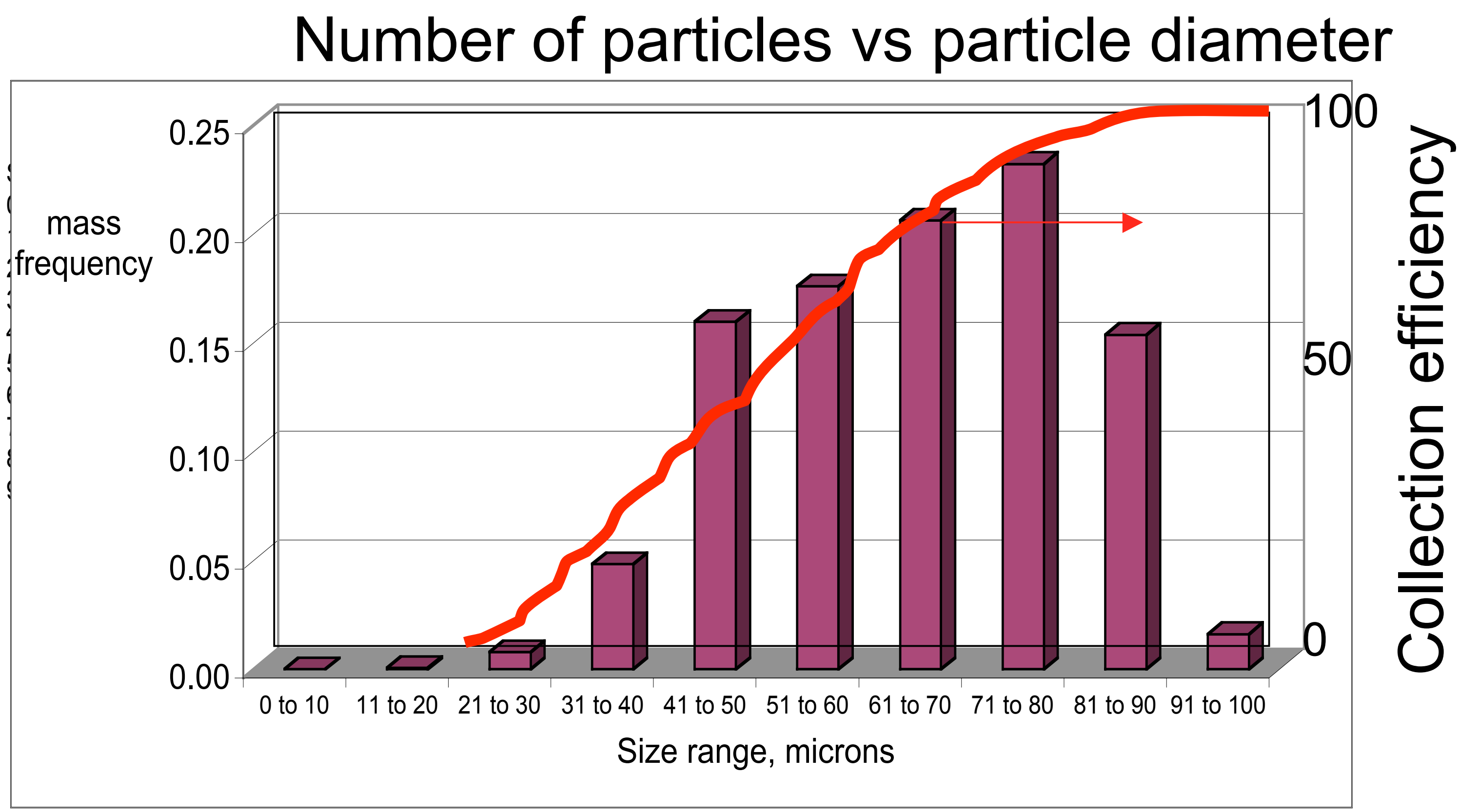
- Advantages
  - Low pressure drop
  - Cheap to build /maintain (no moving parts)
- Disadvantages
  - Poor efficiency for smaller particles (less than 10 microns)
  - Not suitable for abrasive particles
- Hence, grow particles with agglomerator to increase efficiency

Collection efficiency

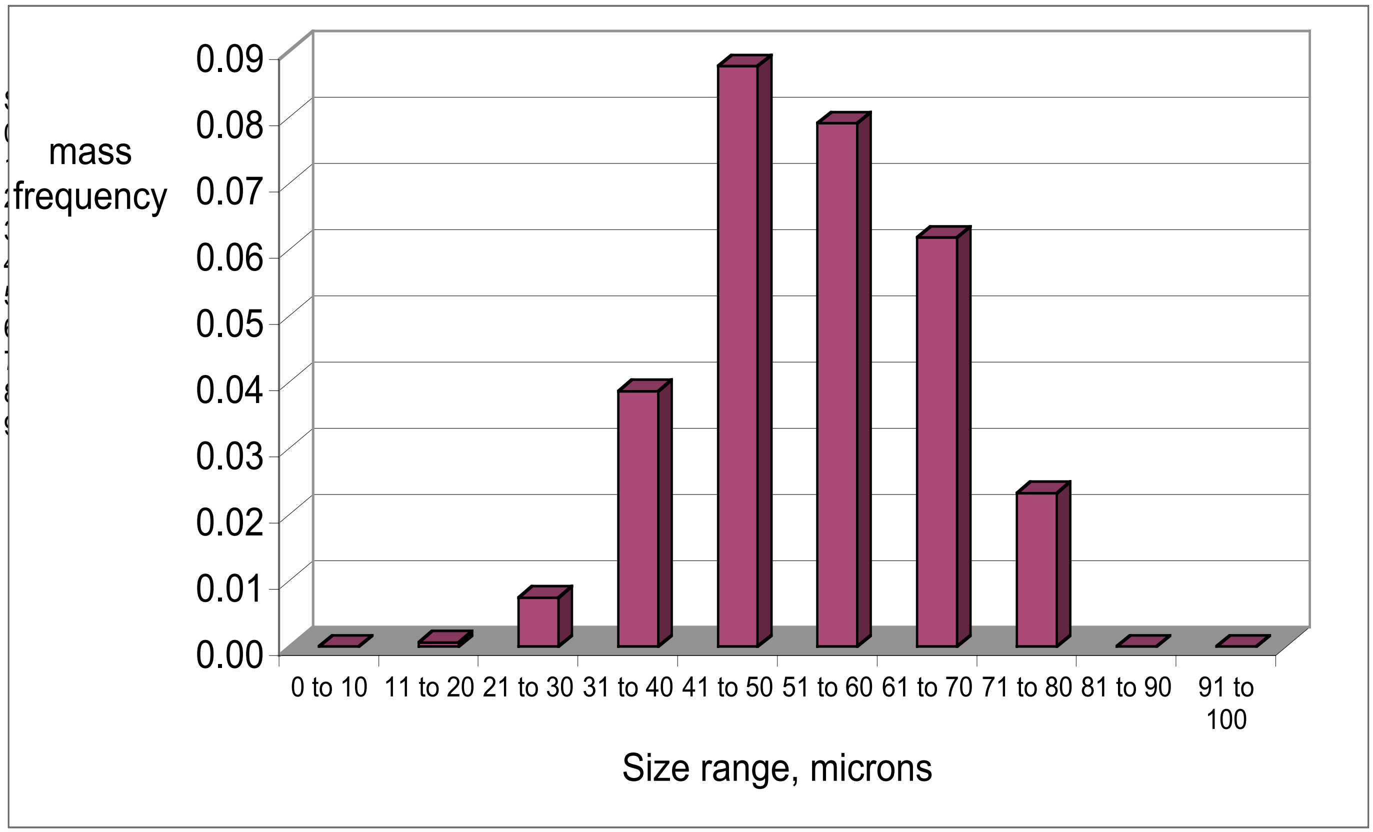
- Example curve



Histogram before cyclone

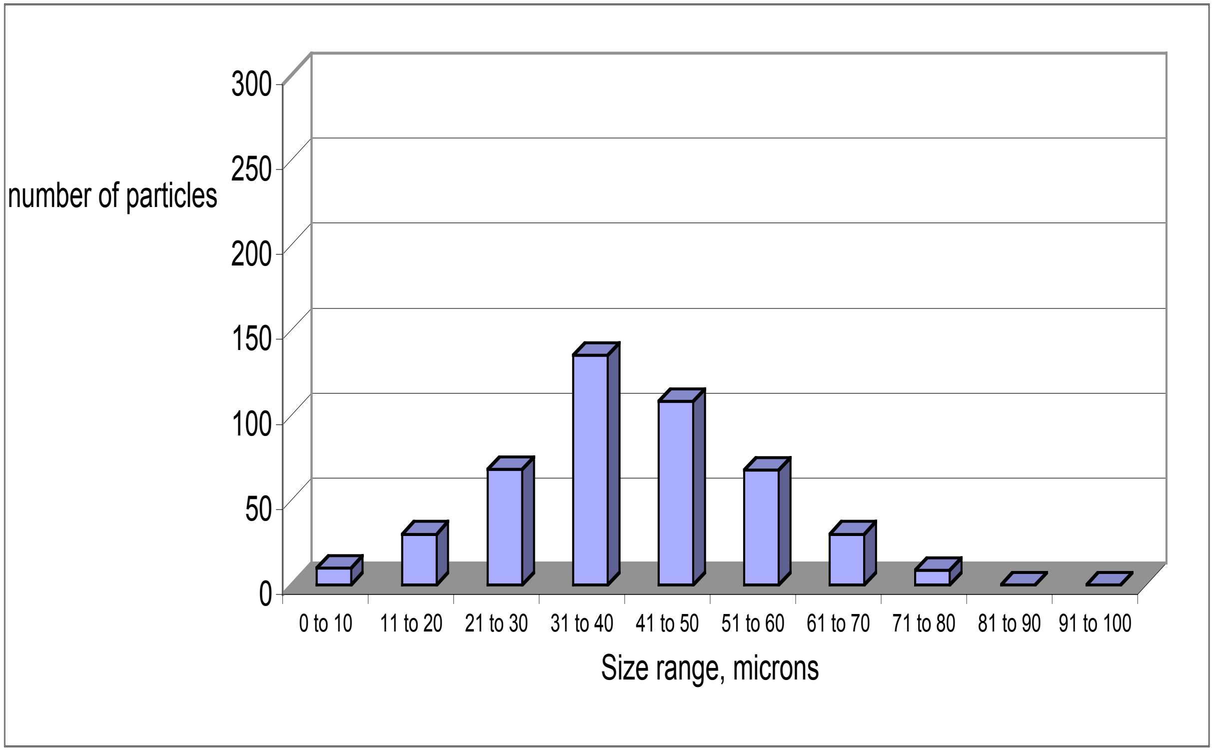


After cyclone



Histogram after cyclone

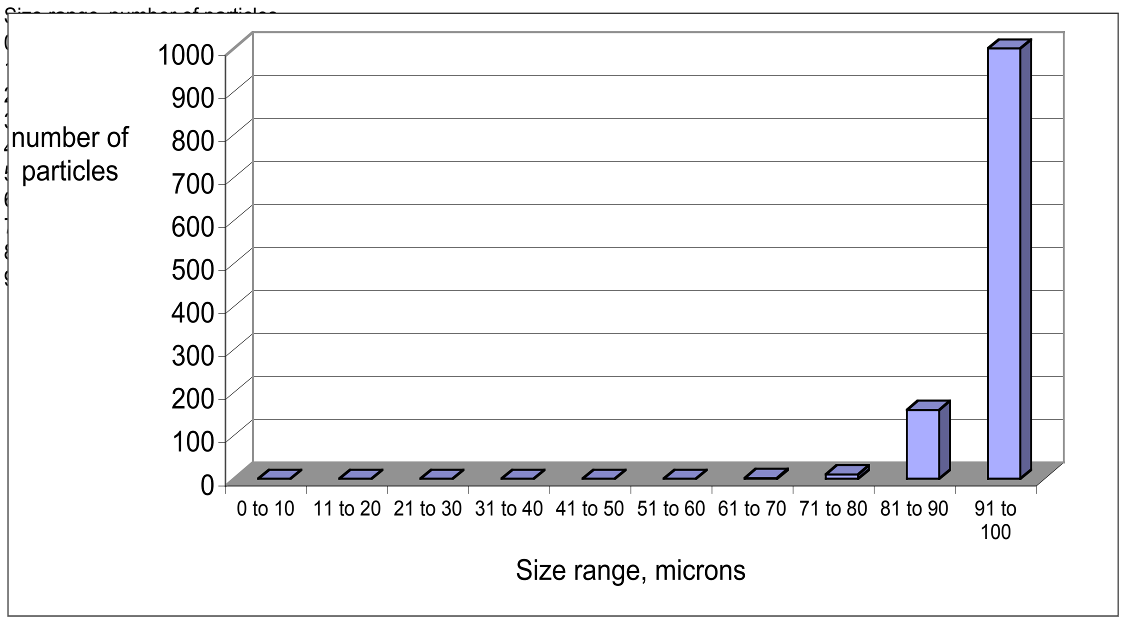
Number of particles vs particle diameter



.

Quick solution?

- Why not make the tube very very long, and just allow a very very long time for coagulation so that the particles become very big?

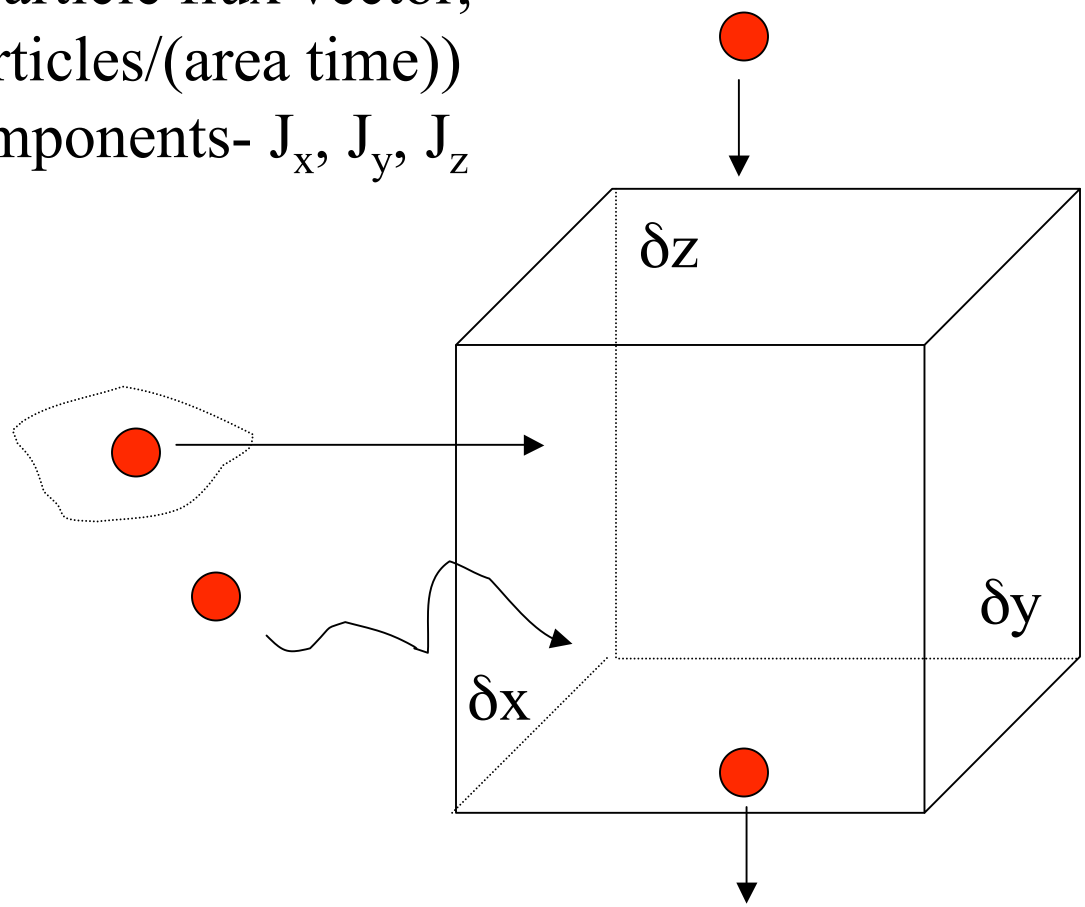


Dynamics of size distributions

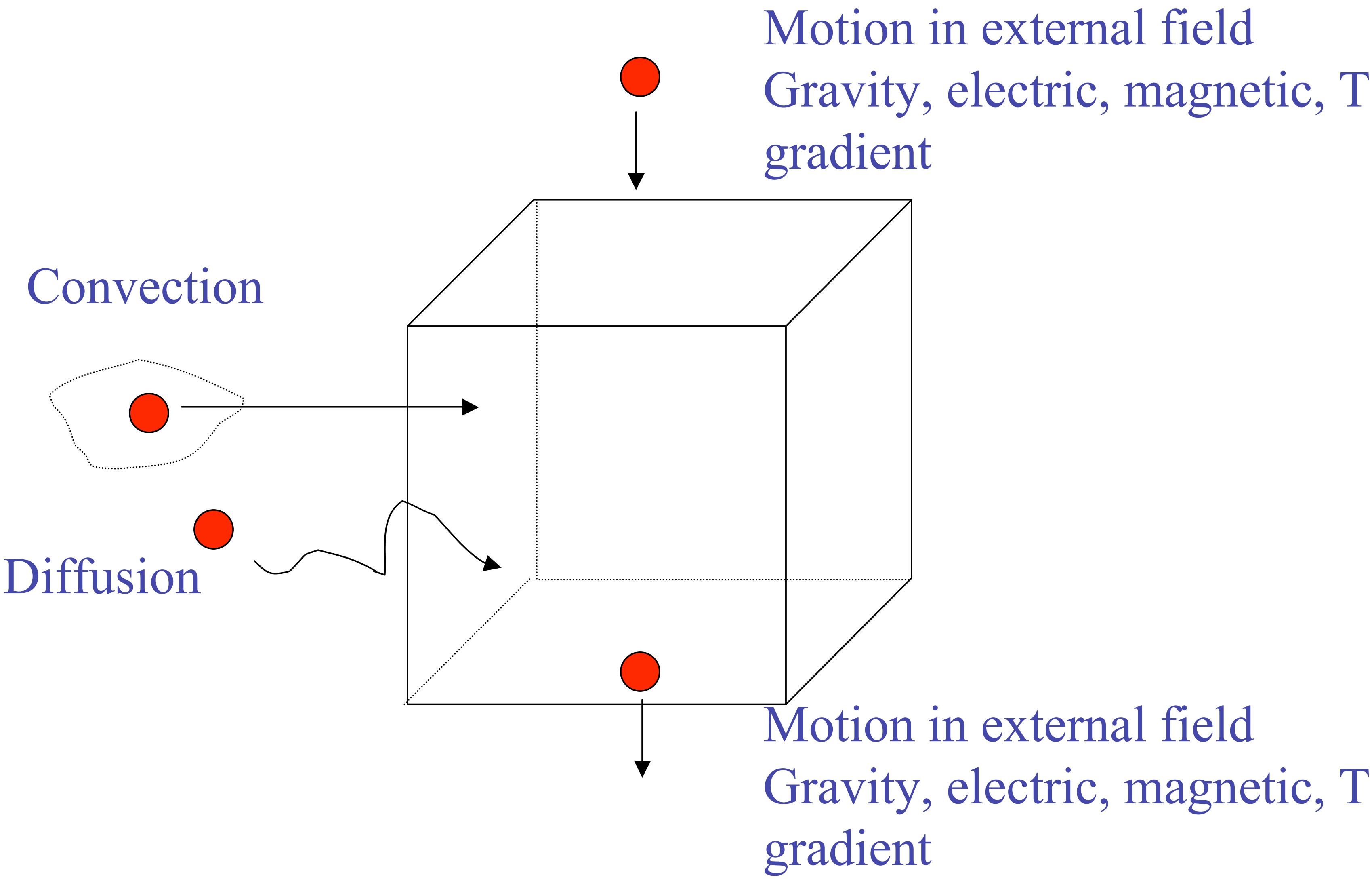
- Control volume approach
- Population balance
- Physics of coagulation/breakup

Take a control volume….

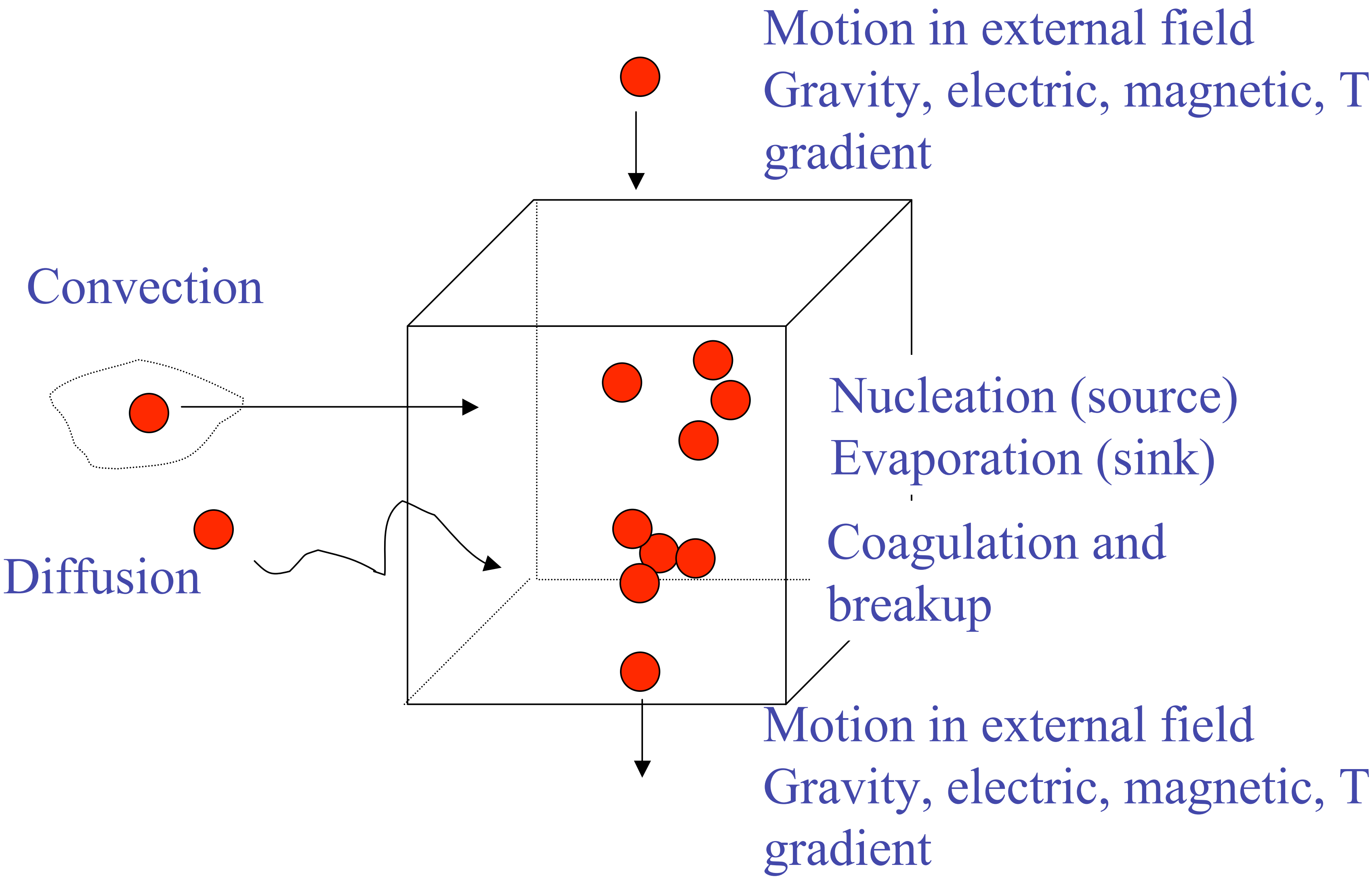
J, particle flux vector, (particles/(area time))
Components- J_x, J_y, J_z



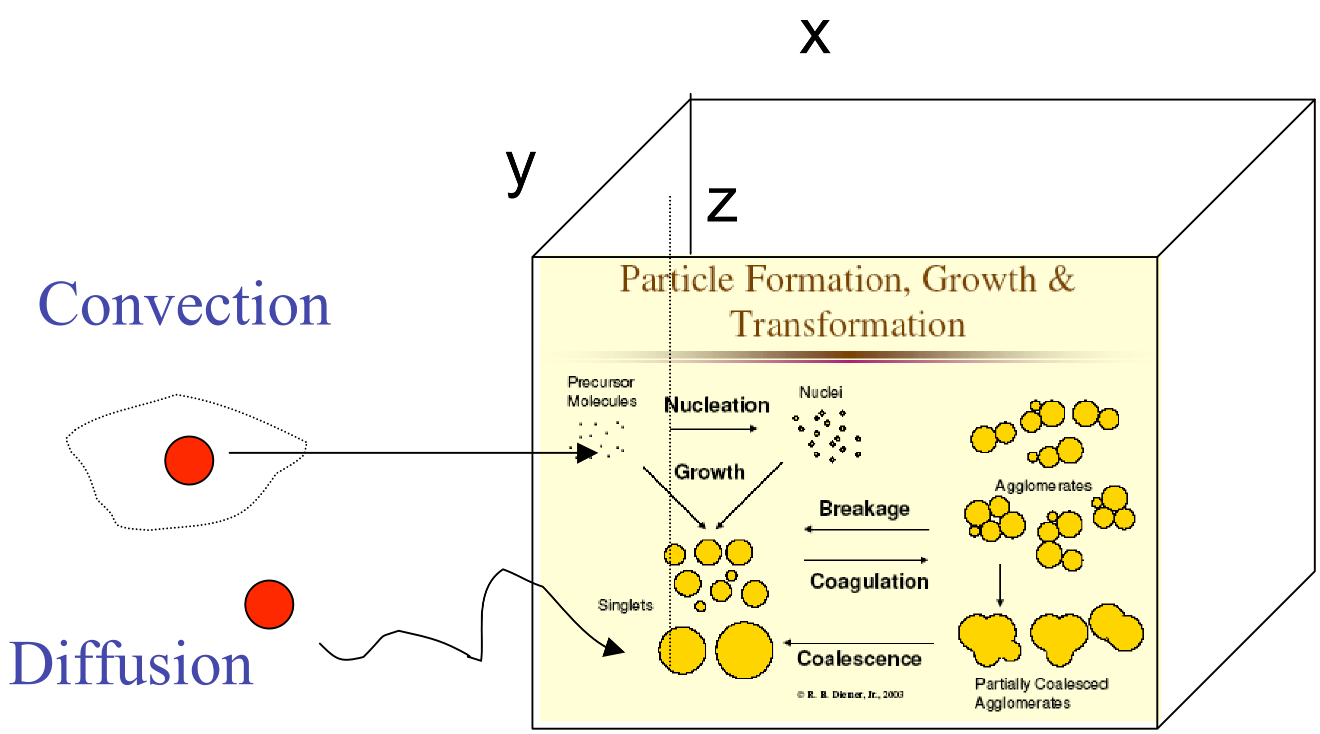
Take a control volume….



Take a control volume….



Take a control volume….



In our problem, no external fields
External coordinates, x,y,z,t
Internal coordinate - particle volume V for 1D population balance

Population balance for dynamics of distributions

- One dimension
  - **Particles, variable diameter**
  - Polymers, variable molecular weight
- 2 dimensions
  - Particles, variable diameter, surface area
  - Polymers, variable molecular weight, number of branch points

Simplifying assumptions, initial conditions

- Assumptions:
  - Steady state, axisymmetric flow, incompressible fluid
  - Plug flow, no slip condition at wall
  - Diffusive transport of particles negligible with respect to convective transport
  - Dynamics of size distribution only varying with axial distance in agglomerator
  - No sources or sinks
- Initial conditions:
  - Particles all same size to start
  - Well mixed

General Differential Form, 1-D Population

$$-\nabla \cdot \left[\mathbf{u}_p(V,\mathbf{x},t)\, n(V,\mathbf{x},t) \right]$$ convection

$$+\nabla \cdot \left[D_p(V,\mathbf{x},t) \nabla n(V,\mathbf{x},t) \right]$$ diffusion

} "In – Out" in external coordinates

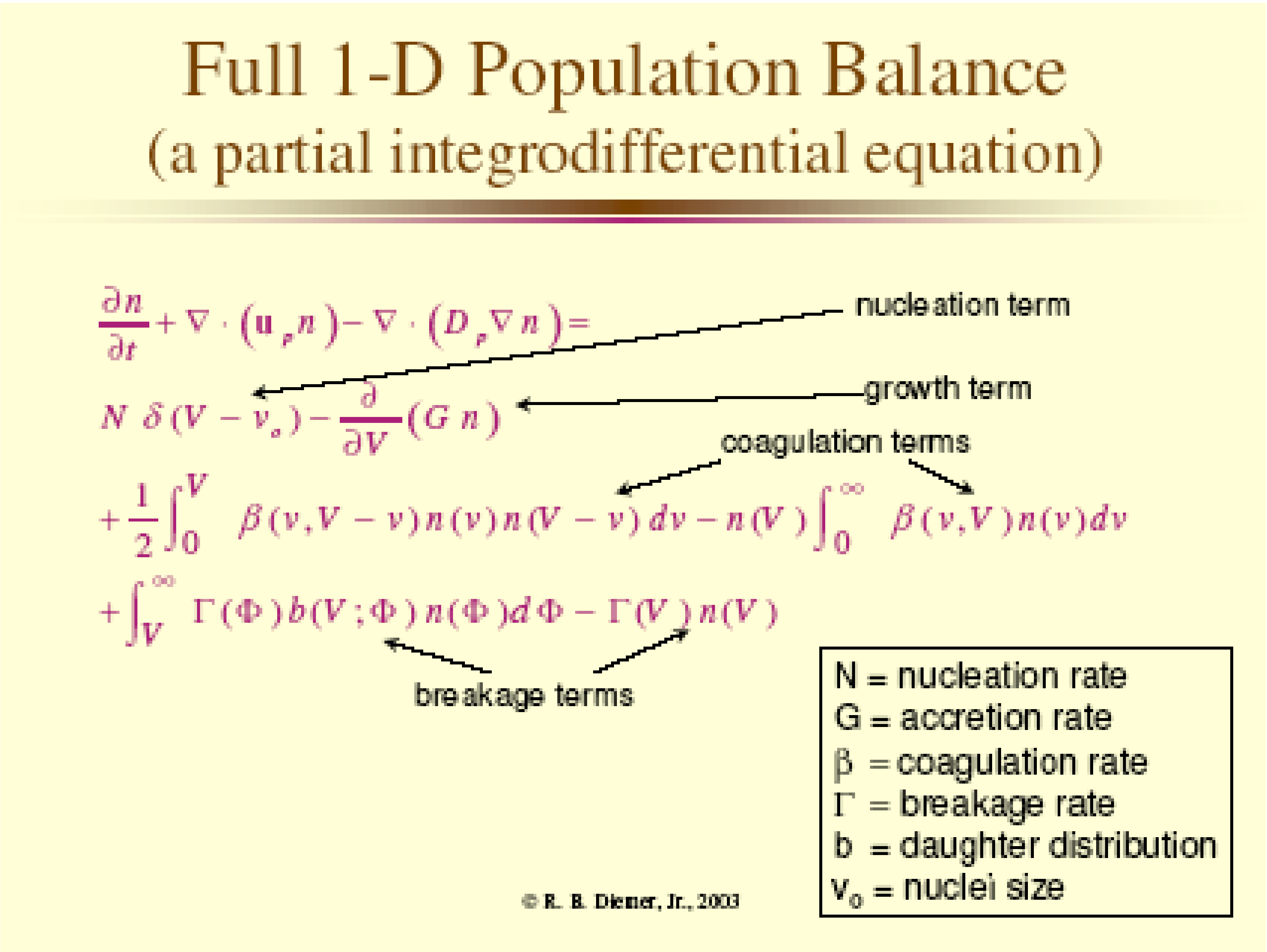
$$-\frac{\partial}{\partial V}\left[G(V,\mathbf{x},t)\, n(V,\mathbf{x},t) \right]$$ growth ("In – Out" in internal coordinate)

$$+S(V,\mathbf{x},t)$$ sources & sinks (Net Generation)

$$=$$

$$\frac{\partial n(V,\mathbf{x},t)}{\partial t}$$ accumulation

Note: object's velocity may differ from fluid's velocity owing to either slip or action of external forces


Full 1-D Population Balance
(a partial integrodifferential equation)
$\frac{\partial n}{\partial t} + \nabla \cdot (\mathbf{u}_p n) - \nabla \cdot (D_p \nabla n) =$
$N\,\delta(V - v_o) - \frac{\partial}{\partial V}(G\,n)$
$+ \frac{1}{2}\int_0^V \beta(v, V - v)\,n(v)\,n(V - v)\,dv - n(V)\int_0^\infty \beta(v, V)\,n(v)\,dv$
$+ \int_V^\infty \Gamma(\Phi)\,b(V;\Phi)\,n(\Phi)\,d\Phi - \Gamma(V)\,n(V)$
nucleation term
growth term
coagulation terms
breakage terms
N = nucleation rate
G = accretion rate
β = coagulation rate
Γ = breakage rate
b = daughter distribution
v_0 = nuclei size
© R. B. Diemer, Jr., 2003

Problem Setup

- Steady-state, incompressible, axisymmetric flow
- Plug flow, no slip
- Neglect diffusion
- Population Balance Model:

$$u_z \frac{\partial n}{\partial z} = \int_V^\infty \Gamma(\Phi)\, b(V;\Phi)\, n(\Phi)\, d\Phi - \Gamma(V)\, n(V)$$
$$+ \frac{1}{2}\int_0^V \beta(v, V-v)\, n(v)\, n(V-v)\, dv - n(V)\int_0^\infty \beta(v,V)\, n(v)\, dv$$

Partial List of Techniques

- Discrete Methods
- Sectional Methods

} Will discuss

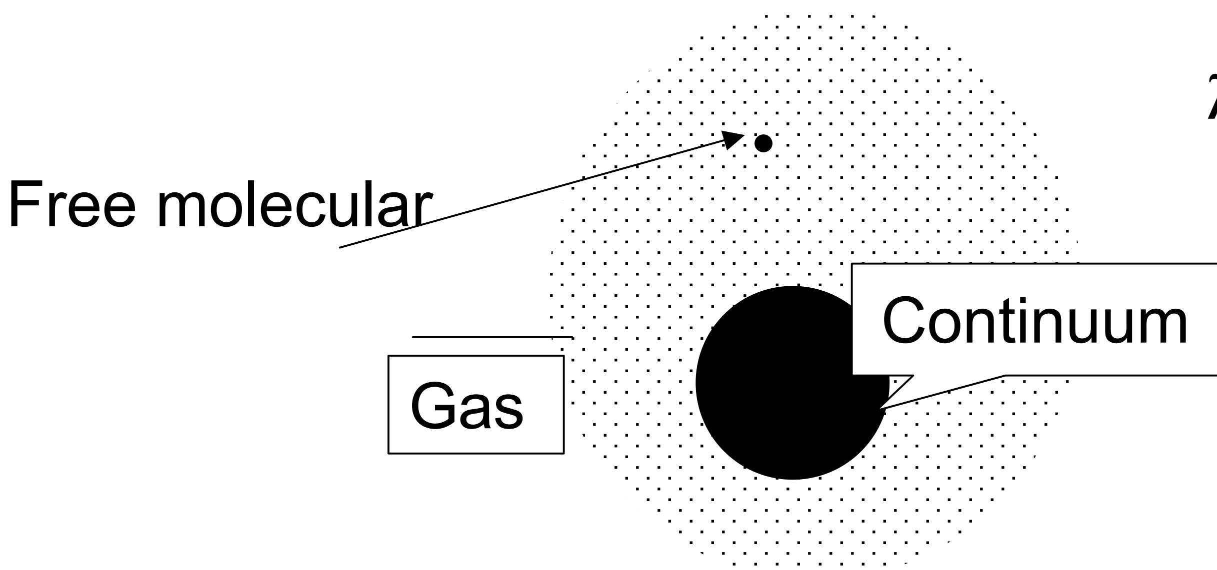
- Similarity Solutions }
- LaPlace Transforms
- Orthogonal Polynomial Methods
- Spectral Methods
- Moment Methods
- Monte Carlo Methods

} Will not discuss

But first, some particle physics

New dimensionless numbers
Knudsen number = $2\lambda/d_p$
Particle Reynolds number = $\rho_f d_p U/\mu$

Free molecular regime: Kn >>1
Continuum regime: Kn <<1
Transition regime: in between



λ -Gas Mean Free Path in air of order 10^{-7} m @STP, U velocity of particle relative to fluid, ρf, fluid density, μ fluid viscosity

Particles in fluid

- So for small particles, collisions with individual gas molecules affect particle motion, growth dynamics

- If size scale of particles --> size scale of eddies in very turbulent flow, turbulence in fluid may affect motion and growth dynamics
  – Levich (1962) agglomeration rate α v_{basic}^9/4
  – Important for particles greater than 1 micron and up

Coagulation - definitions

- Coagulation of solid particles = agglomeration
- When relative motion of particles is Brownian, process = thermal coagulation
- Relative motion from particle- fluid interactions = turbulent coagulation
- Saffman Turner (1956) divided into 2 processes
  - Turbulent shear agglomeration: particles on different streamlines are traveling at different speeds, enhances collisions
  - Turbulent inertial agglomeration: particle trajectories depart from flow streamlines, and lead to collisions

Collision frequency function

Consider the change in number concentration of particles of size i, where $v_i = v_j + v_{i-j}$

collision frequency - # collisions/time between particles of size j and size i-j =

v_i, v_{i-j} are volumes of particles of size j and i- j

$$N_{j,i-j} = \beta\left(v_j, v_{i-j}\right) n_j, n_{i-j}$$

β, also known as a collision kernel, depends on the size of the colliding particles, and properties of system such as temperature

For our problem, we assume all collisions ‘stick’

Test yourself….

- For small particles (free molecular and continuum) will the collision kernel increase or decrease as the system temperature increases?
- For particles in the continuum regime, will the collision kernel increase or decrease as the viscosity of the surrounding gas increases?

Coagulation - discrete distribution bookkeeping

For a discrete size distribution, the rate of formation of particles of size i by collision of particles of size j and i-j, is given by:

$$\frac{1}{2}\sum_{j=1}^{i-1} N_{j,\,i-j}$$

where the factor 1/2 is introduced because each collision is counted twice in summation

Rate of loss of particles of size i by collision with all other particles is given by:

$$\sum_{j=1}^{\infty} N_{i,j}$$

Change in number concentration of particles of size i given by:

$$\frac{dn_i}{dt} = \frac{1}{2}\sum_{j=1}^{i-1} N_{j,i-j} - \sum_{j=1}^{\infty} N_{i,j} = \frac{1}{2}\sum_{j=1}^{i-1} \beta_{j,i-j}(v_{j,}v_{i-j})n_j n_{i-j} - n_i \sum_{j=1}^{\infty} \beta_{ij}(v_{j,}v_i)n_j$$

theory of coagulation for discrete spectrum developed by Smoluchowski (1917) change = formation - loss

Notation change:

Impt for problem statement: Alternate, more general, way to represent two colliding particles, v_j v_{i-j} -->

ϕ, $V-\phi$ where V is final size of pair after collisions

Coagulation, continuous distributions

continuous nomenclature

n(v) = number of particles per unit volume of size v, a continuous distribution

collision rate:

$$N_{\phi,v-\phi} = \beta(\phi,\ v - \phi)\mathrm{n}(\phi)\mathrm{n}(\mathrm{v} - \phi)\mathrm{d}\phi \mathrm{d}(\mathrm{v} - \phi)$$

where β is the collision frequency function described earlier

The rate of formation of particles of size v by collision of smaller particles of size ϕ and v-ϕ is given by:

$$\textit{formation} \text{ in range dv} = \frac{1}{2}\left[\int_0^v \beta(\phi, v-\phi)\mathrm{n}(\phi)\mathrm{n}(v-\phi)\mathrm{d}(\mathrm{v} - \phi)\right]\mathrm{d}v$$

$$\textit{l}\text{oss in range dv} = \left[\int_0^\infty \beta(\phi, v)\mathrm{n}(\phi)\mathrm{n}(v)\mathrm{d}\phi\right]\mathrm{d}v$$

Here, loss is from collisions with all other particles, so must integrate over entire size range

Collision frequency functions

for particles in continuum regime: (Stokes-Einstein relationship valid)

$$\beta(\phi, V-\phi) = \frac{2kT}{3\mu}\left[2 + \left(\frac{\phi}{V-\phi}\right)^{1/3} + \left(\frac{V-\phi}{\phi}\right)^{1/3}\right]$$

for particles in
free molecular regime: (derived from kinetic theory of collisions between hard spheres)

$$\beta_{ij} = \left(\frac{3}{4\pi}\right)^{1/6}\left(\frac{6kT}{\rho_p}\right)^{1/2}\left(\frac{1}{\phi} + \frac{1}{v-\phi}\right)^{1/2}\left(\phi^{1/3} + (v-\phi)^{1/3}\right)^2$$

interpolation formulas between regimes given by
Fuchs (1964) *The Mechanics of Aerosols*

Collision frequency values:

d_1/d_2	0.01	0.1	1.0
		$10^{10}\beta$	cm^3/sec
0.01	18		
0.1	240	14.4	
1.0	3200	48	6.8

where particle diameters, d_1 and d_2 are in microns

Test yourself…

- Why are the collision kernel values greater for collisions between smaller and larger particles compared to particles of the same size?

Turbulent coagulation

$$\beta(\phi, V - \phi) = 0.31\sqrt{\frac{\varepsilon}{\nu}}\left[V + 3\phi^{1/3}(V - \phi)^{2/3} + 3\phi^{2/3}(V - \phi)^{1/3}\right]$$

- ν = kinematic viscosity
- ε = energy dissipation rate (rate of conversion of turbulence into heat by molecular viscosity, m^2/s^3)

Comparison… brownian vs. turbulent

- For collisions between 1 micron diameter particles, Brownian kernel ~ 100 x turbulent kernel
- But for collisions between 500 micron diameter particles, turbulent kernel ~ 10 x Brownian kernel

Breakup

- Definitions:
  - Parent: starting agglomerate, size Φ
  - Daughter: resulting fragments, size V
- Different causes of breakup
  - Thermal/Brownian
  - Flow induced
- Simplifying assumption for our problem
- Breakup into equal sized daughter fragments (size V), rate given by:

$$\Gamma(V) = \Gamma_o \left(\frac{\varepsilon}{\nu} \right)^{3/2} V^{1/3}$$

$$b(V;\Phi) = 2\delta\left(V - \frac{\Phi}{2} \right)$$

Discrete Methods

- Size is integer multiple of fundamental size
- Write balance equations for every size
- Gives distribution directly
- Huge number of equations to solve
- Have to decide what the largest size is
- Example for coagulation and breakage:

$$V_i = iV_0\,; \quad V_0 = \frac{\pi d_0^3}{6}$$

$$u_z \frac{dn_i}{dz} = \frac{1}{2}\sum_{j=1}^{i-1} \beta_{j,i-j} n_j n_{i-j} - n_i \sum_{j=1}^{\infty} \beta_{i,j} n_j + \sum_{j=i+1}^{\infty} \Gamma_j b(i;j) n_j - \Gamma_i n_i$$

Discrete Example Problem Setup

$$\beta_{c,i,j} = \frac{2kT}{3\mu}\left[2+\left(\frac{i}{j}\right)^{1/3}+\left(\frac{j}{i}\right)^{1/3}\right];\quad \beta_{t,i,j} = .31\sqrt{\frac{\varepsilon}{\nu}}V_0\left(i+3i^{2/3}j^{1/3}+3i^{1/3}j^{2/3}+j\right)$$

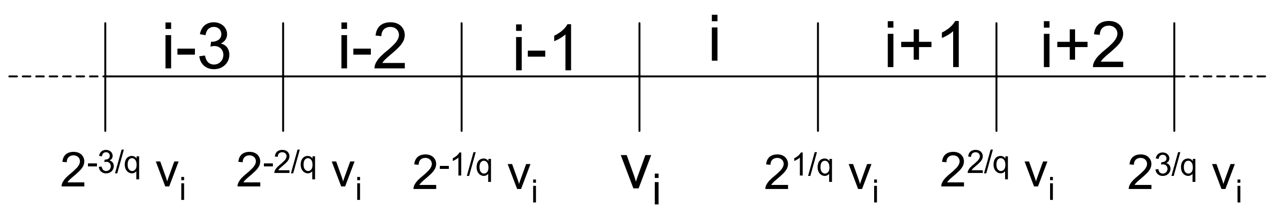
$$\Gamma_i = \begin{cases} 1\times10^{-8}\,\mathrm{s^2/cm}\left(\frac{\varepsilon}{\nu}\right)^{3/2}V_0^{1/3}i^{1/3}, & i>1 \\ 0, & i=1 \end{cases};\quad b(i;j) = \begin{cases} 2, & j=2i \\ 1, & j=2i+1,2i-1 \\ 0, & j<2i-1,\ j>2i+1 \end{cases}$$

$$u_z\frac{dn_i}{dz} = \frac{1}{2}\sum_{j=1}^{i-1}\left(\beta_{c,j,i-j}+\beta_{t,j,i-j}\right)n_j n_{i-j} - n_i\sum_{j=1}^{\infty}\left(\beta_{c,i,j}+\beta_{t,i,j}\right)n_j$$
$$+\Gamma_{2i+1}n_{2i+1}+2\Gamma_{2i}n_{2i}+\Gamma_{2i-1}n_{2i-1}-\Gamma_i n_i$$

Need slightly more than 2×10^6 cells to cover entire mass distribution range!

Sectional Method

- Best rendering due to Litster, Smit and Hounslow
- Collect particles in bins or size classes, with upper/lower size=$2^{1/q}$, “q” optimized for physics



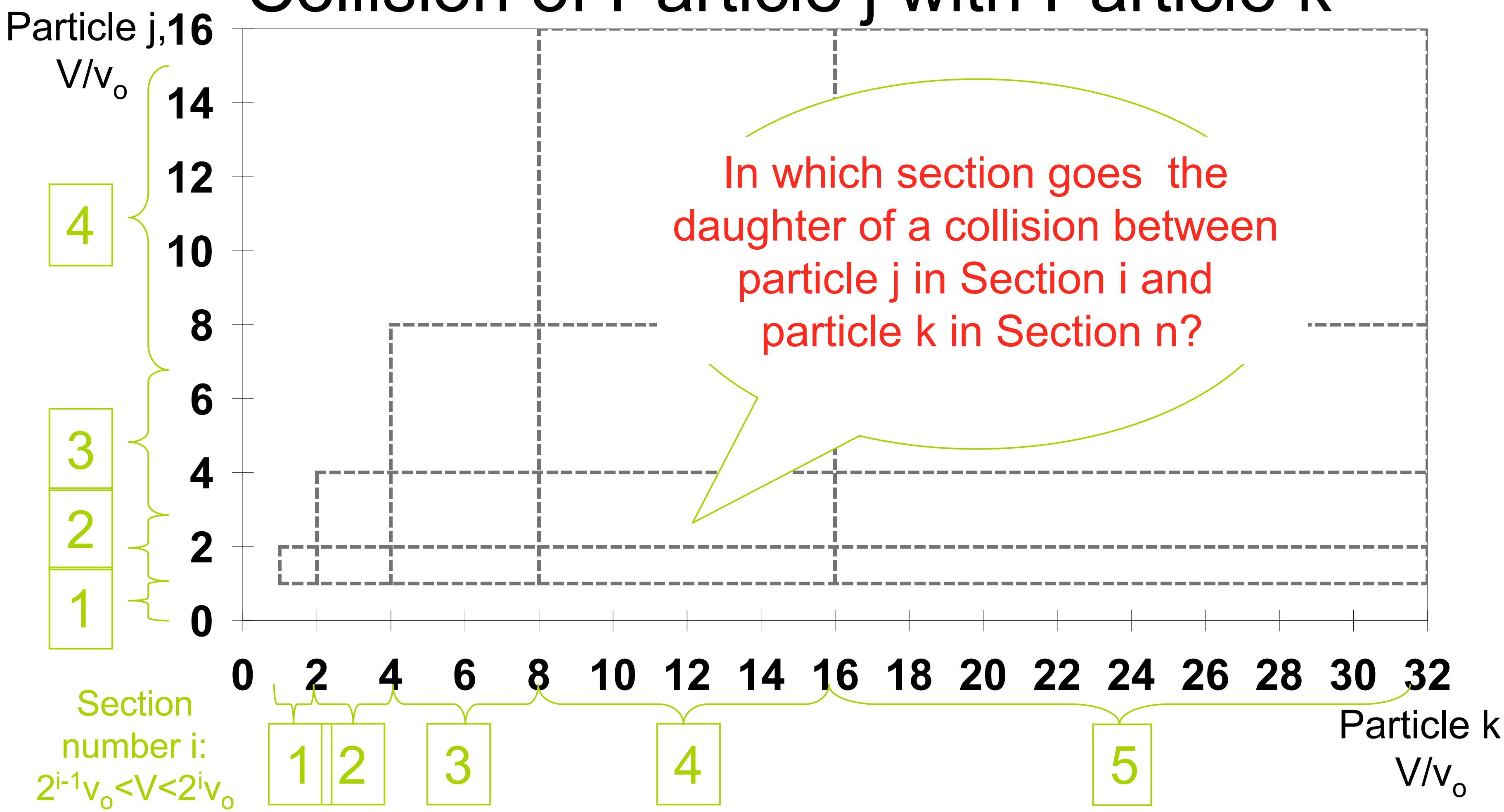
- Balances are written for each size class reducing the number of equations, but too few bins loses resolution
- And… now the equations get more complicated to get the balances right
- Still have problem of growing too large for top class
- Directly computes distribution

Sectional Interaction Types

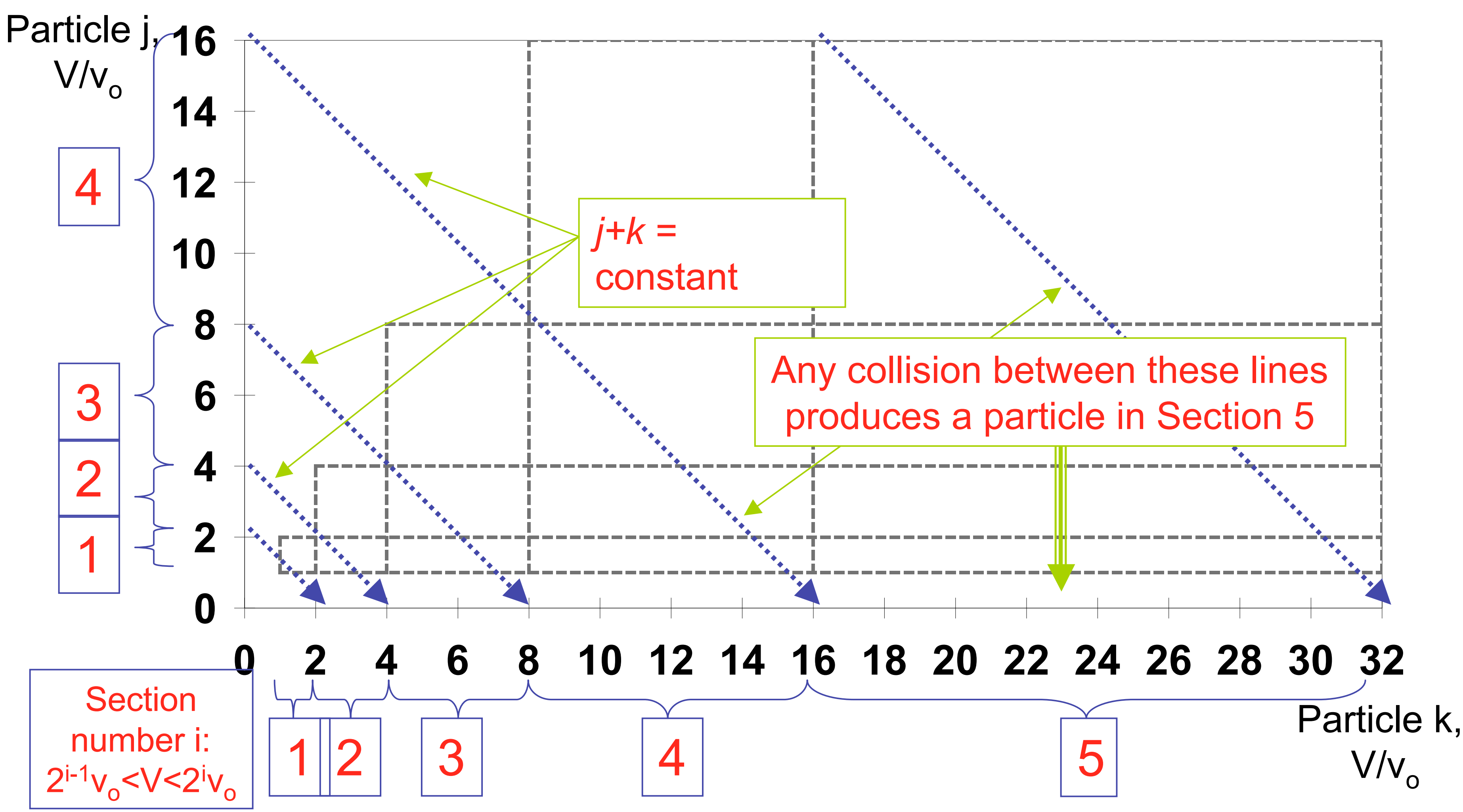
- Type 1:
  - some particles land in the i^{th} interval and some in a smaller interval
- Type 2:
  - all particles land in the i^{th} interval
- Type 3:
  - some particles land in the i^{th} interval and some in a larger interval
- Type 4:
  - some particles are removed from the i^{th} interval and some from other intervals
- Type 5:
  - particles are removed only from i^{th} interval

Sectionalization Example: q=1

Collision of Particle j with Particle k

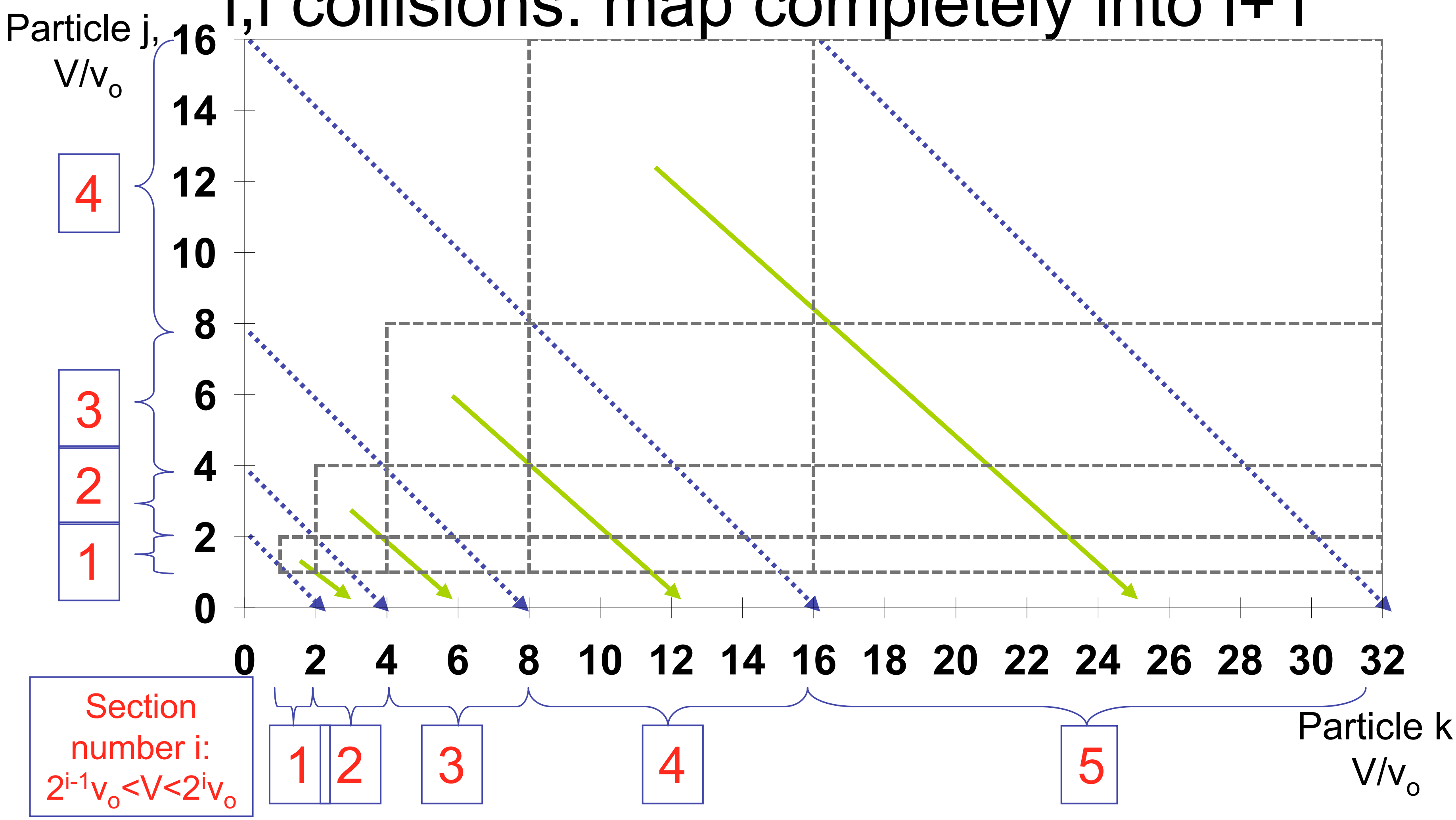


Sectionalization Example: q=1



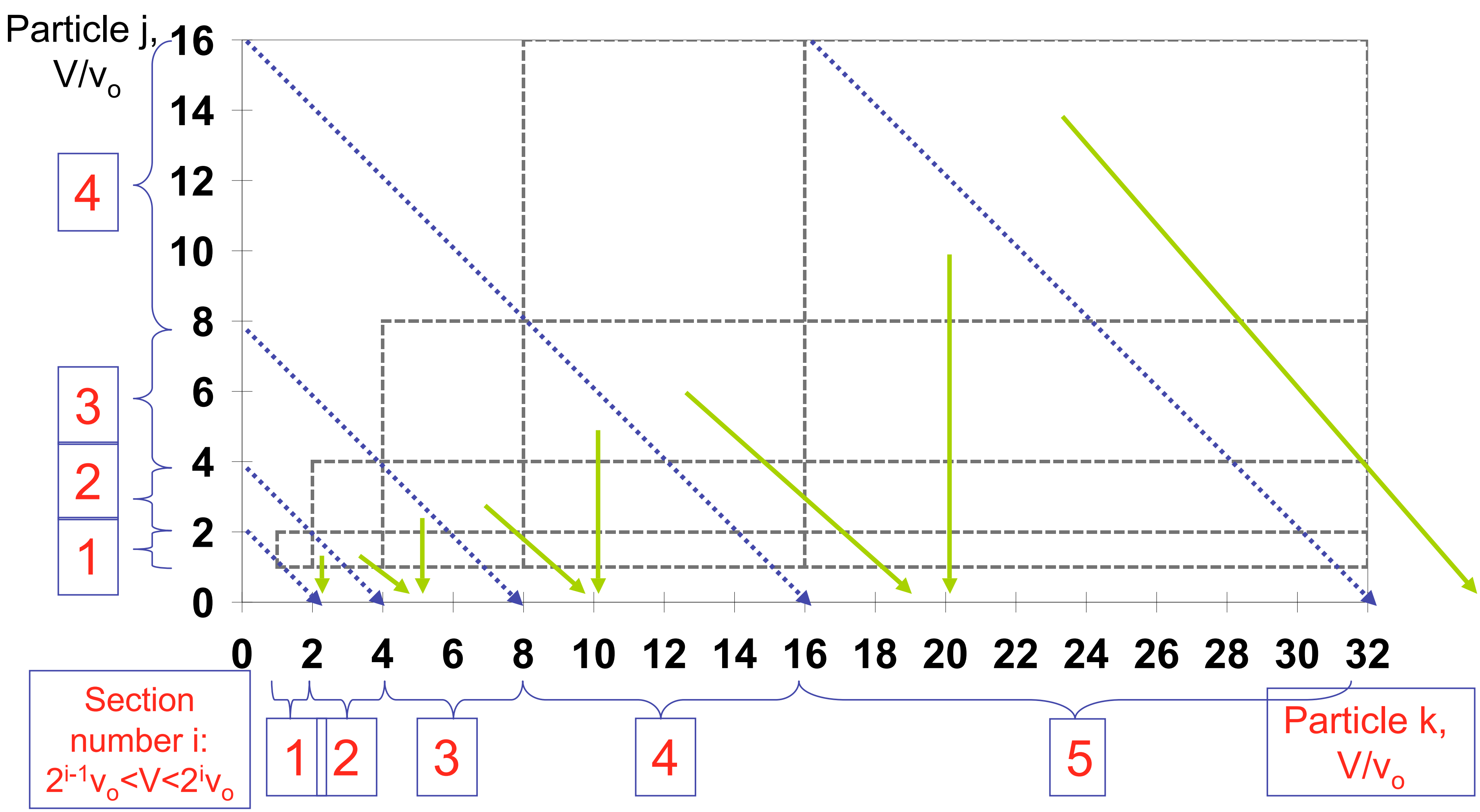
Sectionalization Example: q=1

i,i collisions: map completely into i+1



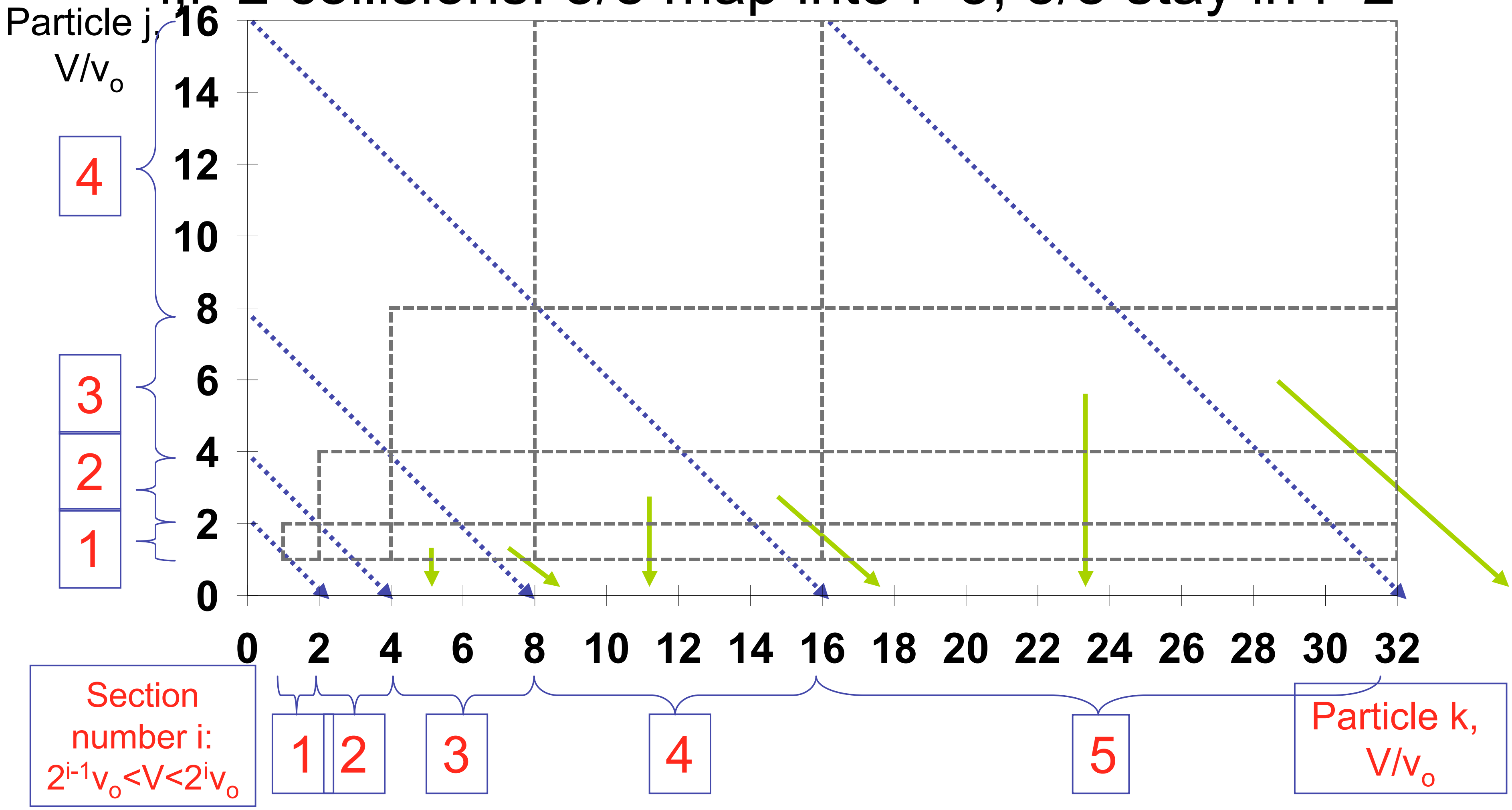
Sectionalization Example: q=1

i,i+1 collisions: 3/4 map into i+2, 1/4 stay in i+1



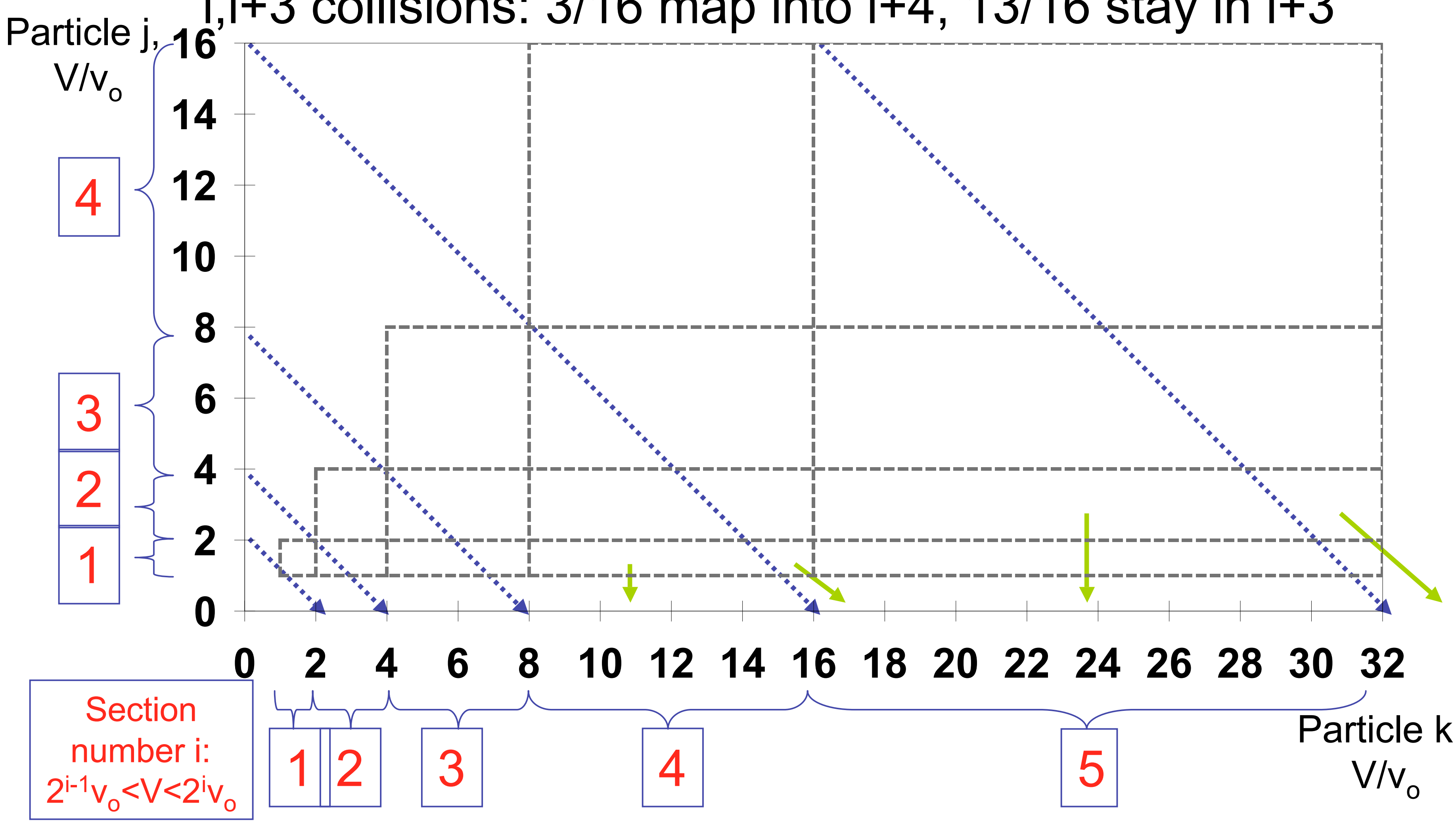
Sectionalization Example: q=1

i,i+2 collisions: 3/8 map into i+3, 5/8 stay in i+2



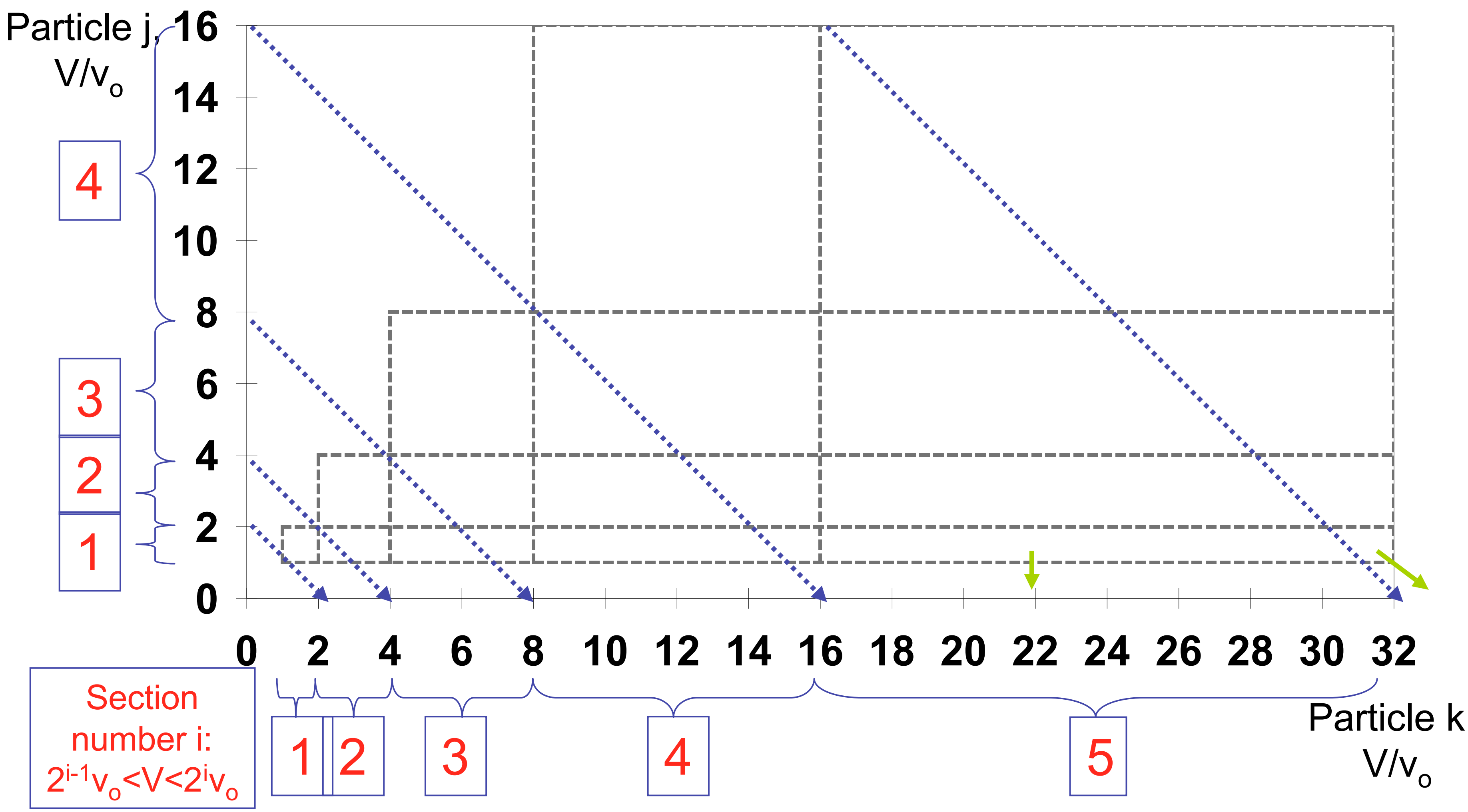
Sectionalization Example: q=1

i,i+3 collisions: 3/16 map into i+4, 13/16 stay in i+3



Sectionalization Example: q=1

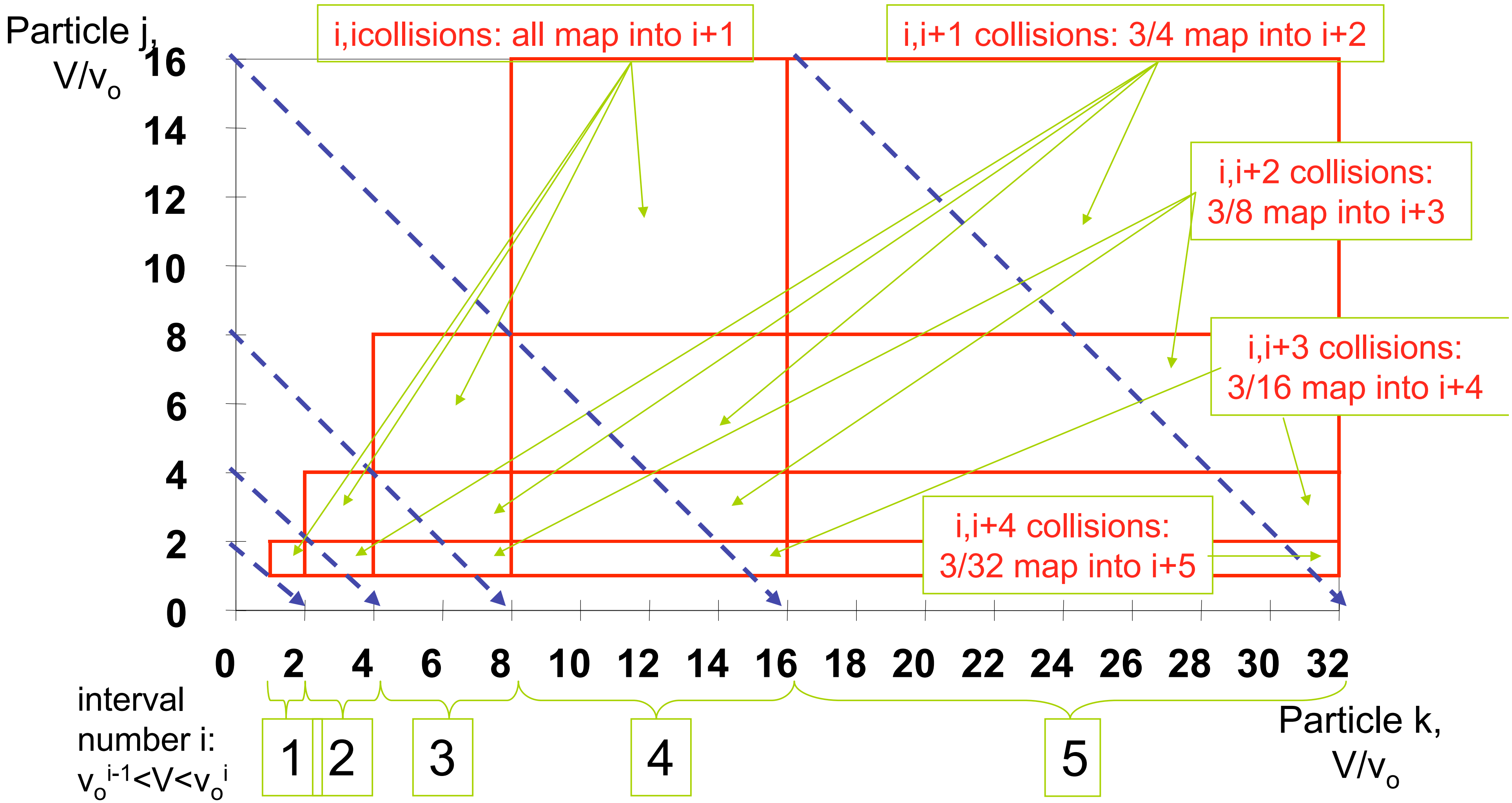
i,i+4 collisions: 3/32 map into i+5, 29/32 stay in i+4



Sectionalization Example: q=1

i,n collisions: $3/2^{n-i+1}$ map into n+1, n>i>0

i,i collisions: all map into i+1



Sectional Coagulation Model, q=1

- Model Equation:

$$u_z \frac{dN_i}{dz} = N_{i-1}\sum_{j=1}^{i-2}\beta_{i-1,j}\theta_{i-1,j}N_j + \frac{1}{2}\beta_{i-1,i-1}N_{i-1}^2 - N_i\left[\sum_{j=1}^{i-1}\beta_{i,j}\theta_{i,j}N_j + \sum_{j=i}^{\infty}\beta_{i,j}N_j\right]$$

- Tentatively:

$$\theta_{i,j} = C\frac{3}{2}2^{j-i}$$

- Can show (via 0^{th} and 1^{st} moments) that:
  - number balance gives correct general form for arbitrary $\theta_{i,j}$
  - mass balance only closes for $C=2/3$ when $V_i/V_j=2^{i-j}$
  - final expression: $\theta_{i,j} = 2^{j-i}$
  - kernels evaluated via:

$$\overline{V}_i = 2^{i-1}\overline{V}_1 \quad \text{with} \quad \overline{V}_1 = \frac{V_0 + 2V_0}{2} = \frac{3V_0}{2} \quad \text{(recovers 3/2 factor)}$$

Gaa!

- At least breakup is easier to visualize
- True equi-sized daughter distributions
- All particles from bin i that breakup will map to lower bin i-1

Sectional Example Problem Setup (for q=1)

$$\beta_{i,j} = \frac{2kT}{3\mu}\left[2 + 2^{(i-j)/3} + 2^{(j-i)/3}\right] + .31\sqrt{\frac{\varepsilon}{\nu}}\left(\frac{3V_0}{2}\right)\left[2^{i-1} + 3\left(2^{(2i+j)/3-1} + 2^{(i+2j)/3-1}\right) + 2^{j-1}\right]$$

$$\Gamma_i = \begin{cases} 1\times10^{-8}\,\mathrm{s}^2/\mathrm{cm}\left(\frac{\varepsilon}{\nu}\right)^{3/2}\left(\frac{3V_0}{2}\right)^{1/3} 2^{(i-1)/3}, & i > 1 \\ 0, & i = 1 \end{cases}; \quad b(i;j) = \begin{cases} 2, & j = i+1 \\ 0, & j \neq i+1 \end{cases}$$

$$u_z \frac{dN_i}{dz} = N_{i-1}\sum_{j=1}^{i-2}\frac{\beta_{i-1,j}}{2^{i-j-1}}N_j + \frac{1}{2}\beta_{i-1,i-1}N_{i-1}^2 - N_i\left[\sum_{j=1}^{i-1}\frac{\beta_{i,j}}{2^{i-j}}N_j + \sum_{j=i}^{\infty}\beta_{i,j}N_j\right]$$
$$+2\Gamma_{i+1}N_{i+1} - \Gamma_i N_i$$

Need about 22 sections to cover entire mass distribution range, suggest using 25-30

General $2^{1/q}$ Sectional Coagulation Model

$$\frac{dN_i}{dt} = N_{i-1}\sum_{j=1}^{i-S(q)-1}\beta_{i-1,j}\theta_{i-1,j}N_j + \frac{1}{2}\beta_{i-q,i-q}N_{i-q}^2 - N_i\left[\sum_{j=1}^{i-S(q)}\beta_{i,j}\theta_{i,j}N_j + \sum_{j=i-S(q)+1}^{\infty}\beta_{i,j}N_j\right]$$

$$\left.\begin{aligned} &+\sum_{k=2}^{q}\sum_{j=i-S(q-k+2)-k+1}^{i-S(q-k+1)-k}\beta_{i-k,j}\left(\theta_{i-1,j}+\psi_k\right)N_{i-k}N_j \\ &-\sum_{k=2}^{q}\sum_{j=i-S(q-k+2)-k+2}^{i-S(q-k+1)-k+1}\beta_{i-k+1,j}\left(\theta_{i,j}+2^{1/q}\psi_{k+1}\right)N_{i-k+1}N_j \end{aligned}\right\} \text{ 2 new terms}$$

$$S(q)=\sum_{m=1}^{q}m;\quad \theta_{i,j}=\frac{2^{(j-i)/q}}{2^{1/q}-1};\quad \psi_k=\frac{2^{(1-k)/q}-1}{2^{1/q}-1}$$

Sectional Example Problem Setup (for q=1)
Nondimensionalization

$$\beta_{i,j} = \beta_c^o \Psi_{c,i,j} + \beta_t^o \left(\frac{3V_0}{2}\right) \Psi_{t,i,j}; \quad \Gamma_i = \Gamma^o \left(\frac{3V_0}{2}\right)^{1/3} 2^{(i-1)/3}$$

$$\beta_c^o = \frac{2kT}{3\mu}; \quad \Psi_{c,i,j} = 2 + 2^{(i-j)/3} + 2^{(j-i)/3}; \quad \Gamma^o = 1\times10^{-8}\,\mathrm{s^2/cm}\left(\frac{\varepsilon}{\nu}\right)^{3/2}$$

$$\beta_t^o = .31\sqrt{\frac{\varepsilon}{\nu}}; \quad \Psi_{t,i,j} = 2^{i-1} + 3\left(2^{(2i+j)/3-1} + 2^{(i+2j)/3-1}\right) + 2^{j-1}$$

$$\Theta = \frac{\tau}{\tau_c} = \frac{\beta_c^o M_0^o z}{u_z}; \quad \Theta_t = \frac{\tau_t}{\tau_c} = \frac{2\beta_c^o}{3\beta_t^o V_0}; \quad \Theta_b = \frac{\tau_b}{\tau_c} = \frac{\beta_c^o M_0^o}{\Gamma^o}\left(\frac{2}{3V_0}\right)^{1/3}$$

$$\Psi_{i,j} = \Psi_{c,i,j} + \frac{\Psi_{t,i,j}}{\Theta_t}; \quad n_i = \frac{N_i}{M_0^o}; \quad M_0^o = \frac{2M_1}{3V_0} = \frac{4M_1}{\pi d_0^3}$$

$$\frac{dn_i}{d\Theta} = n_{i-1}\sum_{j=1}^{i-2}\frac{\Psi_{i-1,j}}{2^{i-j-1}}n_j + \frac{1}{2}\Psi_{i-1,i-1}n_{i-1}^2 - n_i\left[\sum_{j=1}^{i-1}\frac{\Psi_{i,j}}{2^{i-j}}n_j + \sum_{j=i}^{\infty}\Psi_{i,j}n_j\right] + \frac{2^{(i-1)/3}}{\Theta_b}\left(2^{4/3}n_{i+1} - n_i\right)$$

Solution tools:

- YOU need to figure out, and modify
  - Change # sections
  - change pipe dimensions
- popbal.m
  - Main, runs functions, checks efficiency, adjusts pipe length till 75% efficiency in cyclone met, checks mass closure
- numdist.m
  - Function, solves ODEs
- gamma.m
  - Function, calculates breakup kernels
- beta.m
  - Function, calculates coagulation kernels

References

1. Nelson, R. D.; Davies, R.; Jacob, K., Teach -em particle technology. *Chemical Engineering Education* **1995,** 29, (1), 12-15.
2. Litster, J. D.; Smit, D. J.; Hounslow, M. J., Adjustable discretized population balance for growth and aggregation. *AIChE Journal* **1995,** 41, (3), 591-603.
3. Diemer, R. B.; Ehrman, S. H., Pipeline agglomerator design as a model test case. *Powder Technology* **2005,** 156, 129-145.

Embedded spreadsheet for histogram

Size range, microns	number of particles	Frequency	assume diameter	mass of particles in each bin, g	Mass frequency
0 to 10	10	0.01	5	6.54E-10	0.00
11 to 20	30	0.03	15	5.30E-08	0.00
21 to 30	80	0.08	25	6.54E-07	0.01
31 to 40	180	0.18	35	4.04E-06	0.05
41 to 50	280	0.28	45	1.34E-05	0.16
51 to 60	169	0.169	55	1.47E-05	0.18
61 to 70	120	0.12	65	1.72E-05	0.21
71 to 80	88	0.088	75	1.94E-05	0.23
81 to 90	40	0.04	85	1.29E-05	0.15
91 to 100	3	0.003	95	1.35E-06	0.02

total number	1000				
total mass assuming 1g/cc density				8.37E-05	

Number frequency vs particle diameter