PHEN 612

SPRING 2008
WEEK 12
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Mixing in Reactors

Agitation, Mixing of Fluids and Power requirements

- ***Agitation*** and ***mixing*** are two of the most common operations in the processing industries
- Agitation: the forcing of a fluid material by some mechanical means (i.e., a motor driven agitator) to force the fluid to flow in a circulatory or other pattern in a vessel.
- Mixing: taking two or more separate phases, such as fluid and a powdered solid or two fluids, and causing them to distribute randomly through one another.

Purposes of agitation:

1) Blending of two miscible liquids, such as ethyl alcohol and water
2) Dissolving solids in liquids, such as salt in water
3) Dispersing a gas in a liquid a fine bubbles (oxygen in fermentation)
4) Suspending solid particles in a liquid (e.g., catalyst particles and hydrogen bubbles dispersed in a liquid)
5) Agitation of the fluid to increase heat transfer between the fluid and a coil and jacket in a vessel wall

Mixing in Reactors

Equipment for Agitation:

- Generally, liquids are agitated in a cylindrical vessel which can be either closed or open to the atmosphere. An impeller mounted on a shaft is driven by an electric motor.

1) Three-blade propeller agitators (400 to 1750 rpm). Used for liquids of low viscosity. The flow pattern in a baffled tank is axial. See **Fig. 3.4.1** in handout.

2) Paddle agitators (20 to 200 rpm). Total length of paddle: 60-80% of tank diameter. Width of blade: 1/6 to 1/10 of its length. At high speeds, baffles promote mixing. Anchor or gate paddle is often used with viscous fluid where deposits on wall can occur since this type of paddle scrapes tank wall and sometimes tank bottom. See **Figs. 3.4.2 a and 3.4.2 b** in handout.

3) Turbine agitators. Used at high speed for liquids with a very wide range of viscosities. Diameter of a turbine is between 30 to 50% of the tank diameter. Flat blades and pitched-blades are used. Flat blade **(Fig. 3.4.2 c** in handout**)** : radial flow and good gas dispersion. Pitched-blade **(Fig. 3.4.2 d)** : axial and radial flow: suspending solids.

4) Helical-ribbon agitators: used for highly viscous solutions. Low RPM. The liquids move in a tortuous flow path down the center and up along the sides in a twisting motion (**Fig. 3.4.4** in handout).

Mixing in Reactors

- Agitator selection and viscosity ranges:
  - Propellers: below about 3 Pa.s (3000 cp)
  - Turbines: below about 100 Pa.s (100,000 cp)
  - Anchor agitators: 50 Pa.s (50,000 cp) to 500 Pa.s (500,000 cp)
  - Helical and ribbon-type agitators: 500 Pa.s (500,000 cp) to 1000 Pa.s (1,000,000 cp) and up to 25,000 Pa.s.
  - For viscosity greater than 2.5 to 5 Pa.s, baffles are not needed since we have little swirling above these viscosities.

Mixing in Reactors

Type of flow in an agitated vessel depends

- Type and diameter of the impeller
- Characteristics of the fluid: density, viscosity, Newtonian or non-Newtonian.

Generally, <u>three distinct flow patterns</u> in an agitated vessel resulting from the 3 components of the fluid velocity:

- radial component acting perpendicular to the centrally located revolving shaft.
- longitudinal component acting parallel to the centrally located revolving shaft.
- tangential, or rotational, component acting tangential to the end of the impeller. The direction is a circular path around the revolving shaft.

- Radial and longitudinal components are desirable for good agitation and mixing. The tangential component can result in a ***vortex:*** swirling in a circular motion, surface of liquid at the shaft moves downward toward the impeller, liquid level at the wall increases. This condition is not desirable for good mixing. Baffles at the vessel wall are installed to present a vortex.

Mixing in Reactors

- **Power used in Agitated Vessels**
  - To design an agitated vessel, we need to estimate the power required to drive the impeller.
  - Reynolds number $$N_{RE}^{'} = \frac{Da_a^2 N \rho}{\mu}$$
  - D_a: impeller (agitator) diameter (m)
  - N: rotational speed (rev/s)
  - ρ: fluid density (kg/m^3)
  - μ: fluid viscosity (kg/m.s)

Laminar flow: $N_{RE}^{'} < 10$

Turbulent flow: $N_{RE}^{'} > 10^4$

Transitional flow: $10 < N_{RE}^{'} < 10^4$

Mixing in Reactors

- Power consumption :

$$N_p = \frac{P}{\rho N^3 D_a^5} \qquad (SI)$$

$$N_p = \frac{P g_c}{\rho N^3 D_a^5} \qquad (English)$$

P is in J/s or W. In English units P is in $\text{ft.lb}_f/\text{s}$

g_c = 32.174 $\text{ft.lb}_m/\text{lb}_f.\text{s}^2$

Use **Fig. 3.4-5 in handout** to estimate the power number (N_p)

Mixing in Reactors

Scale-up procedure:

- **Table 3.4-1** is the handout gives geometric proportions for a “standard” agitation system.
- A step-by-step procedure to follow in the scale-up:
  - Use **Fig 3.4-3 c** to get the dimensions of turbine and tank
  - Calculate the scale-up ratio R. The original vessel is a standard cylinder with $D_{T1} = H_1$, the volume is:

$$V_1 = \left(\frac{\pi D_{T1}^2}{4}\right)(H_1) = \left(\frac{\pi D_{T1}^3}{4}\right)$$

  - Then the ratio of the volume is:

$$\frac{V_2}{V_1} = \left(\frac{\pi D_{T2}^3}{4}\right) \Big/ \left(\frac{\pi D_{T1}^3}{4}\right) = \frac{D_{T2}^3}{D_{T1}^3}$$

  - The scale-up ratio is the:

$$R = \left(\frac{V_2}{V_1}\right)^{1/3} = \frac{D_{T2}}{D_{T1}}$$

  - The new dimensions are (The dimensions are given in Table 3.4-1):

$$D_{a2} = RD_{a1}, \qquad J_2 = RJ_1, ...$$

  - The agitator speed is:

$$N_2 = N_1\left(\frac{1}{R}\right)^n = N_1\left(\frac{D_{T1}}{D_{T2}}\right)^n$$

Knowing N_2, P can be calculated using $N_p = \frac{P}{\rho N^3 D_a^5}$

or Fig. 3.4.5

n=1: equal liquid motion; n=3/4: equal suspension of solid;
n=2/3: equal rates of mass transfer (equal power per unit volume)

Mixing in Reactors

- A tracer can help identify good mixing (i.e., randomness of the distribution)
- In a reactor: Macroelements: have physical dimensions; microelements: no any physical dimension.
- <u>Micro-mixing</u>:

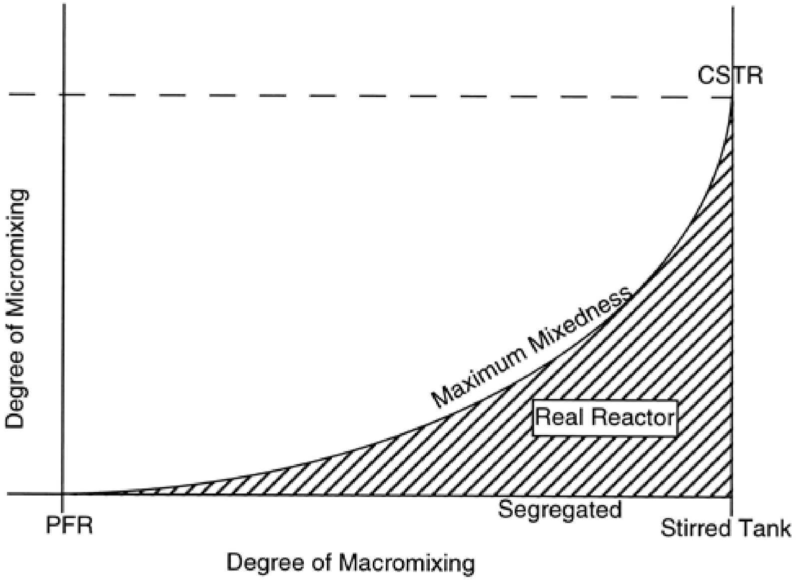
  - Complete segregation: micro-elements, within each macro-element, mix with each other. No crossing boundary

  - maximum mixedness: micro-elements can cross boundaries of macro-elements and mix with other micro-elements. The result is that all macro-elements lose their identity.
- <u>Macro-mixing</u>:
  - Ideal PFR has no macromixing
  - CSTR maximum degree of macromixing

CSTR: segregation and maximum mixedness (for an ideal CSTR).

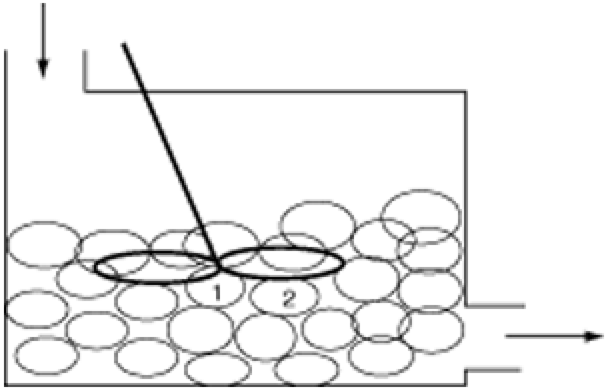
Ideal PFR: both micro-mixing and macro-mixing are absent.

In between we have real reactors.



Mixing in Reactors

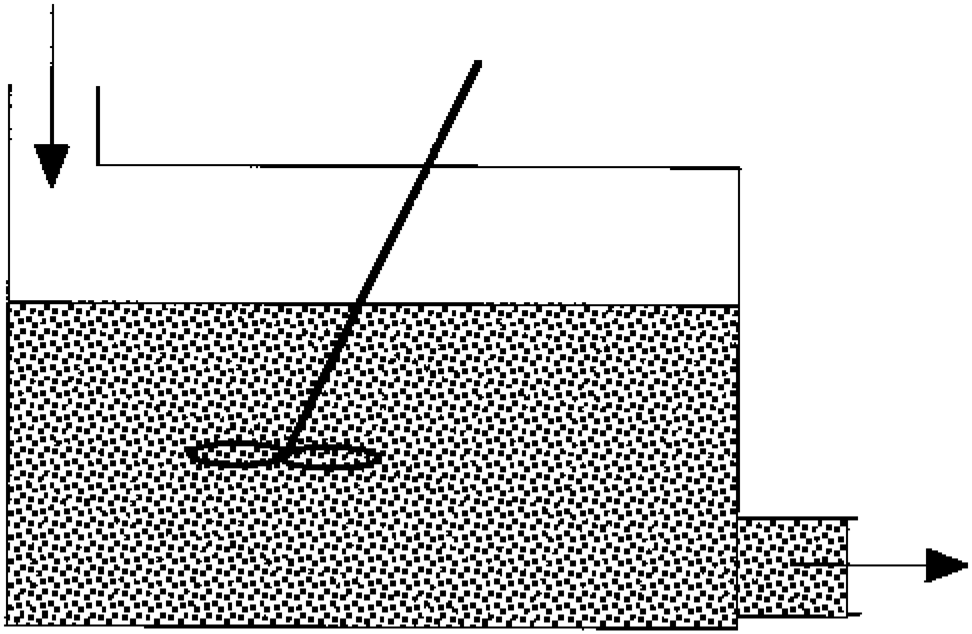
- No exchange of reactants among macroelements
- Complete mixing of micro-elements in each macro-element
- Each macro-element can be viewed as a well-mixed batch reactor



Segregation

Mixing in Reactors

- Complete mixing and exchange of microelements among all macroelements
- Boundaries of all macroelements are not defined



Micro-mixing

Mixing in Reactors

Mixing/reaction interactions

- Before a chemical reaction takes place, the reactants have to be mixed on a molecular scale (i.e., micro-mixing).
- Slow reaction, fast mixing -> Product depends on kinetics
- Fast reaction, slow mixing -> mixing rate influences yield and selectivity
- Model reactions can be used to study the local state of micro-mixing
- The yield can be used as a segregation index

Residence-time Distribution (RTD) – Chapter 13

- RTD of a reactor is a characteristic of the mixing that occurs.
- RTD for plug-flow and CSTR are different.
- A tracer is used: pulse or step injection

Pulse injection

$$\frac{\Delta N}{N_0} = \frac{vC(t)}{N_0}\Delta t$$

Fraction of material exiting that has spent a time between to and t+Δt in the reactor

$$E(t) = \frac{vC(t)}{N_0}; \qquad \frac{\Delta N}{N_0} = E(t)\Delta t$$

E(t) is the residence-time distribution function.

Using: $N_0 = \int_0^\infty vC(t)\,dt$

and constant volumetric flow rate *v:*

$$E(t) = \frac{C(t)}{\int_0^\infty C(t)\,dt}$$

E(t)dt is the fraction of fluid exiting the reactor that has spent between time t and dt inside the reactor.

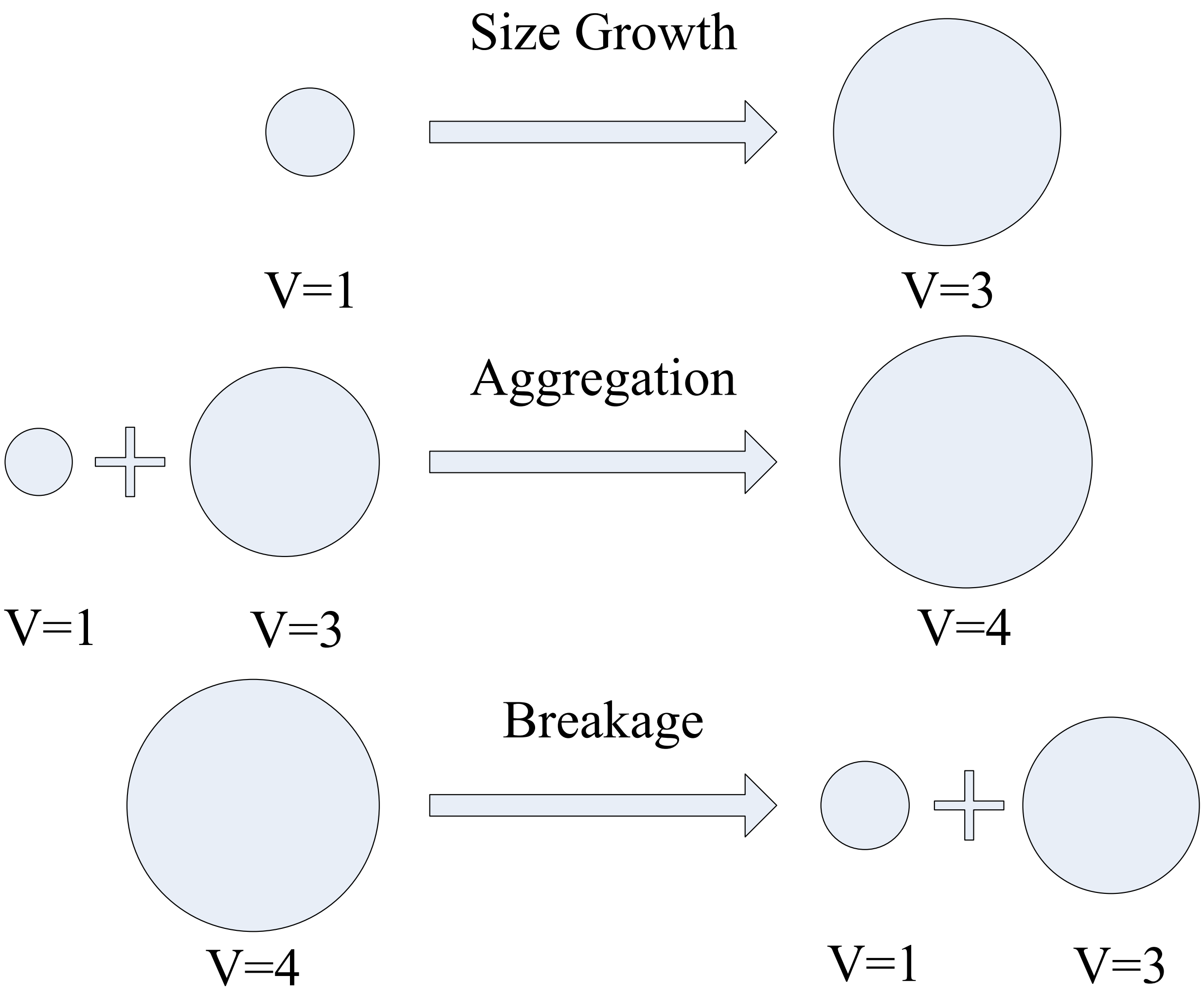
Page 873, example 13-1

Modeling of Nonideal Pharmaceutical Reactors

Mechanisms in Particulate System

- Particle Size Growth
- Aggregation
- Breakage

Each mechanism contributes to the birth and death of particles of all sizes


Size Growth
V=1
V=3
Aggregation
V=1
V=3
V=4
Breakage
V=4
V=1
V=3

Population Balance Equation

$$\frac{\partial n(V,t)}{\partial t}+\frac{\partial\big(G(V)\,n(V,t)\big)}{\partial V}$$

$$=\int_{V_{\min}}^{V/2}\beta(U,V-U)\,n(U,t)\,n(V-U,t)\,dU$$

$$-\,n(V,t)\int_{V_{\min}}^{V_{\max}}\beta(V,U)\,n(U,t)\,dU.$$

Variables & Parameters

t	Time
V	Particle size (volume)
$n(V,t)$	Number density of particle size between V and $V+dV$
$G(V)$	Volume-dependent growth rate
$\beta(U,V)$	Volume-dependent aggregation rate

Results for Case 1

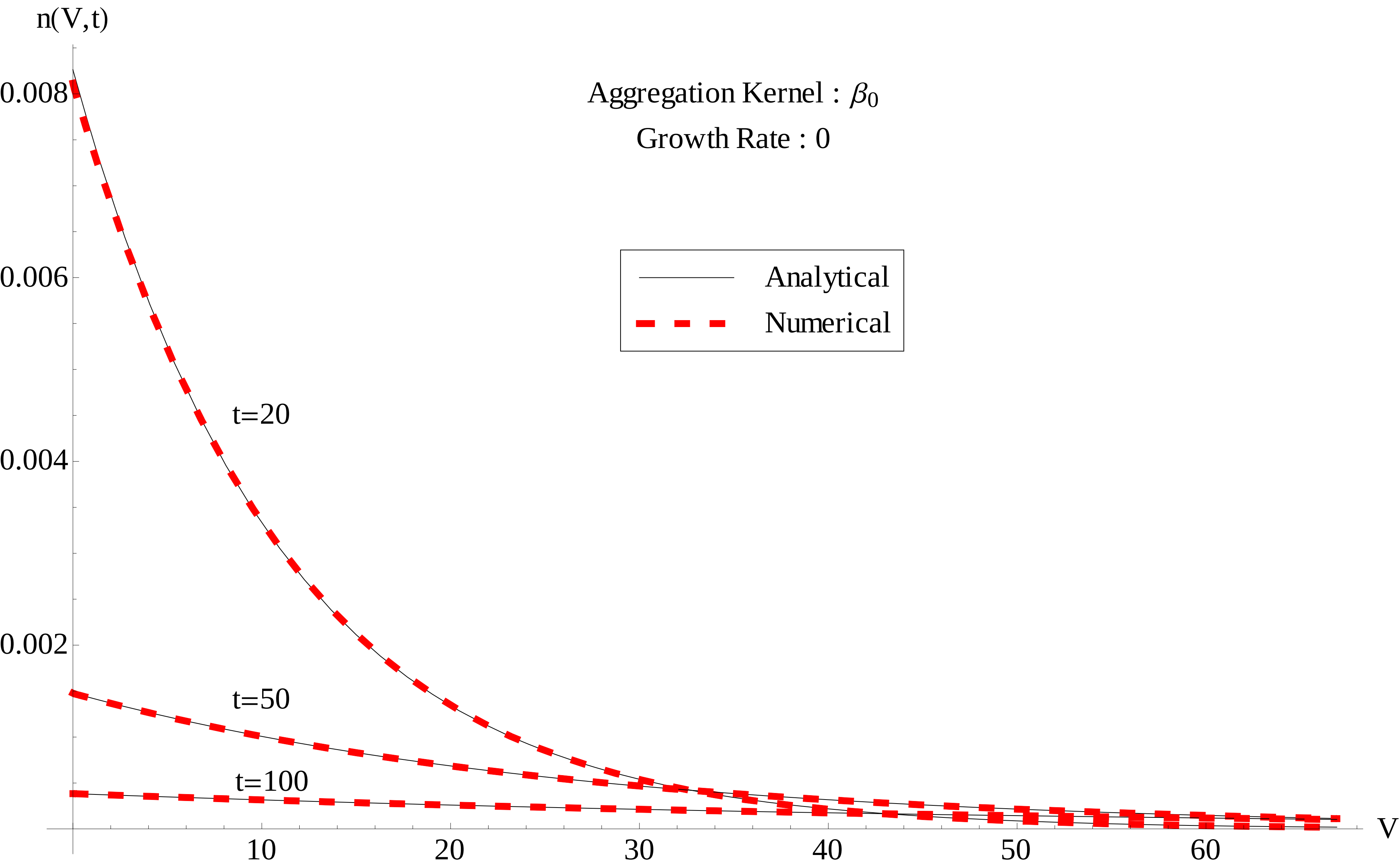
- Simulation conducted using the following parameters:

$$N_0 = 1 \qquad v_0 = 1$$

$$\sigma_0 = 0 \qquad \beta_0 = 1$$

$$G\left(V\right) = 0$$

$$\beta\left(U,V\right) = \beta_0 = 1$$


n(V,t)
0.008
0.006
0.004
0.002
Aggregation Kernel : β_0
Growth Rate : 0
Analytical
Numerical
t=20
t=50
t=100
10
20
30
40
50
60
V

Results for Case 2

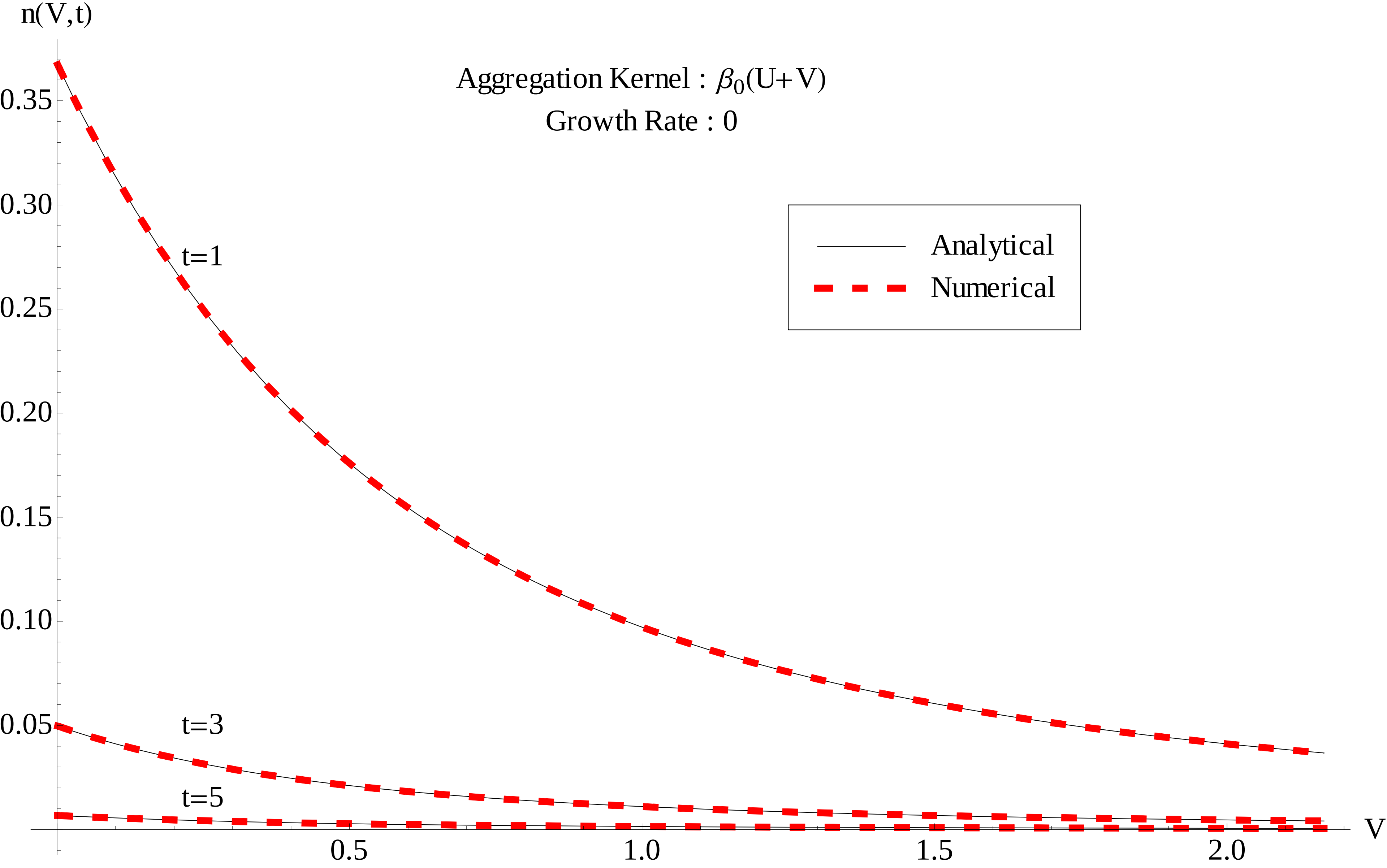
- Simulation conducted using the following parameters:

$$N_0 = 1 \qquad v_0 = 1$$

$$\sigma_0 = 0 \qquad \beta_0 = 1$$

$$G(V) = 0$$

$$\beta(U,V) = \beta_0 (U + V) = U + V$$


n(V,t)
Aggregation Kernel : $\beta_0(U+V)$
Growth Rate : 0
Analytical
Numerical
t=1
t=3
t=5
0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.5
1.0
1.5
2.0
V

Results for Case 3

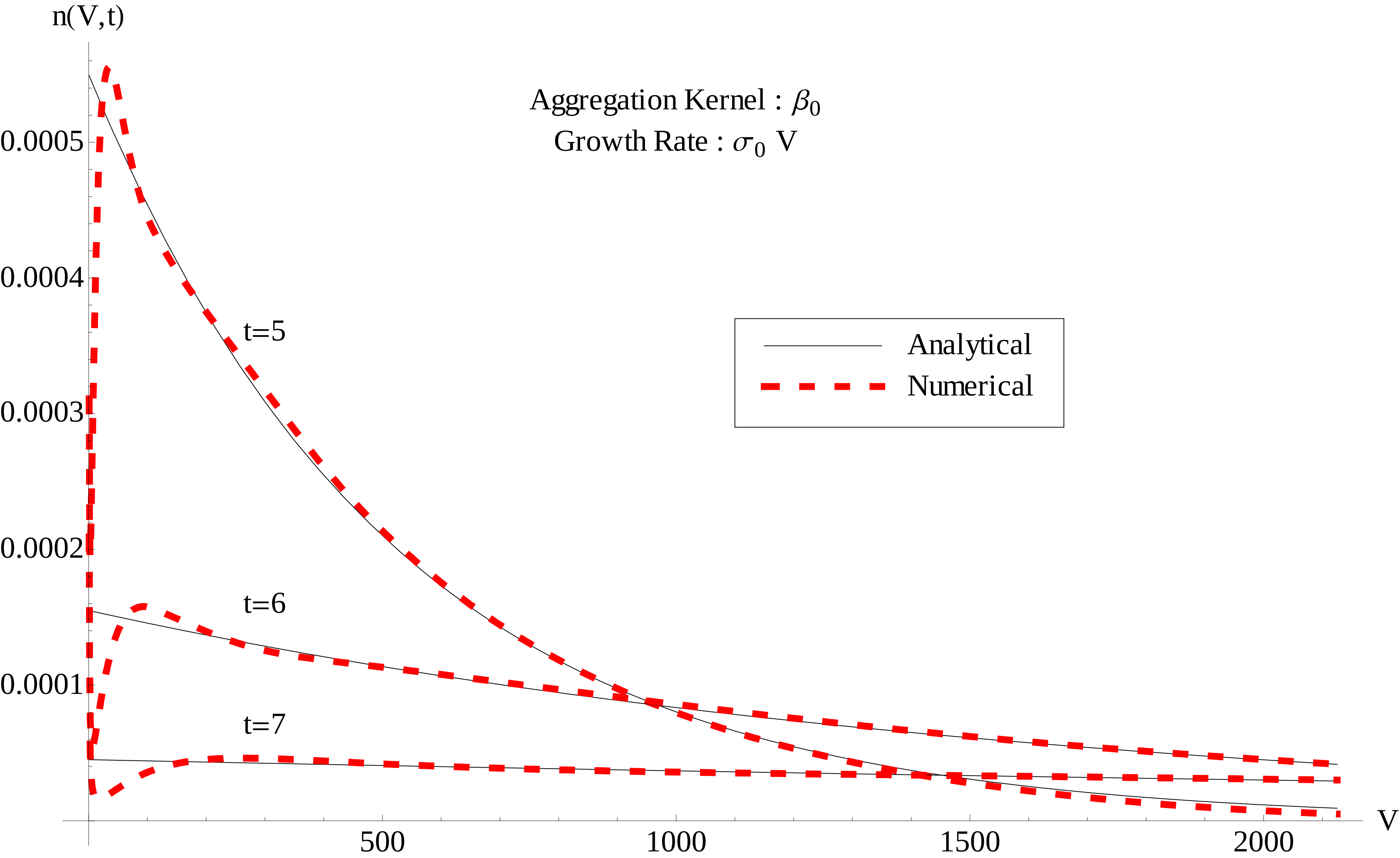
- Simulation conducted using the following parameters:

$$N_0 = 1 \qquad v_0 = 1$$

$$\sigma_0 = 1 \qquad \beta_0 = 1$$

$$G(V) = \sigma_0 \frac{V}{v_0} = V$$

$$\beta(U,V) = \beta_0 = 1$$


n(V,t)
Aggregation Kernel : β_0
Growth Rate : σ_0 V
0.0005
0.0004
0.0003
0.0002
0.0001
t=5
t=6
t=7
Analytical
Numerical
500
1000
1500
2000
V