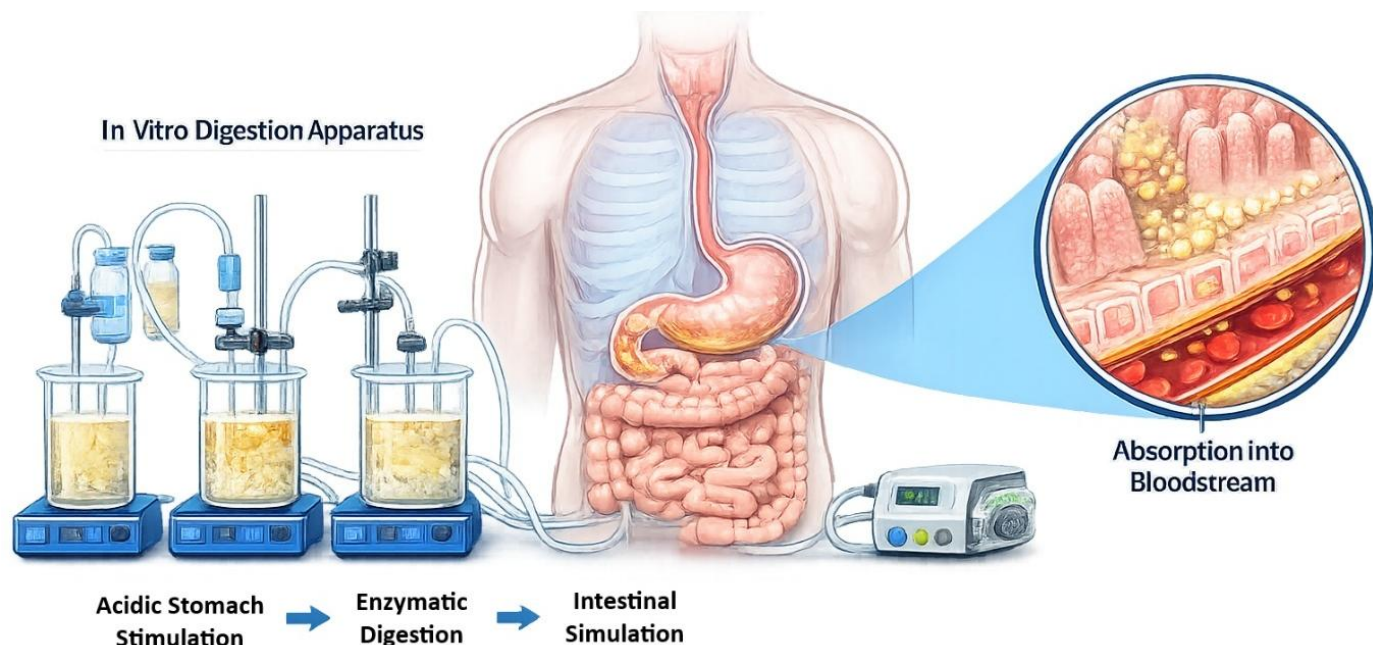


Computer-Aided Biopharmaceutical Characterization

Gastrointestinal Absorption Simulation

- Gastrointestinal (GI) absorption simulation is a computational method used to **predict how a drug is absorbed through the digestive system into the bloodstream.**



What is GI Absorption?

- It is the process by which a drug moves from the stomach and intestines into systemic circulation
- Mainly occurs in the **small intestine** due to large surface area

Why Simulation is Needed

- Real experiments (in vivo) are costly and time-consuming
- Ethical limitations on human and animal testing
- Variability between individuals

Role of Computers

- Simulate drug dissolution, permeability, and transport
- Predict plasma drug concentration profiles
- Evaluate formulation performance

Applications

- Drug development and formulation design
- Predicting food effects
- Supporting regulatory decisions

Common Software Used

- GastroPlus
- Simcyp
- PK-Sim

Advantages

- Reduces need for clinical trials
- Saves time and cost
- Allows testing of multiple scenarios

Theoretical Background of GI Absorption Simulation

- The theoretical basis of GI absorption simulation combines **physiology, drug properties, and mathematical modeling**.

Key processes involved

1. Dissolution

- Drug must dissolve in GI fluids before absorption
- Governed by Noyes–Whitney equation

2. Permeation

- Drug crosses intestinal membrane
- Based on **Fick's law of diffusion**

3. Transit

- Movement of drug through stomach and intestines
- Influenced by gastric emptying and intestinal motility

Key Concepts Involved

ADME Principles

- Absorption
- Distribution
- Metabolism
- Excretion
- Focus here is mainly on **absorption**

Biopharmaceutics Classification System (BCS)

➤ **Drugs are classified based on:**

- Solubility
- Permeability

➤ **BCS Classes**

- Class I: High solubility, high permeability
- Class II: Low solubility, high permeability
- Class III: High solubility, low permeability
- Class IV: Low solubility, low permeability

Fick's Law of Diffusion

- Describes drug movement across membranes
- **Rate of diffusion depends on:**
 - Concentration gradient
 - Surface area
 - Membrane thickness

pH Partition Hypothesis

- Drug absorption depends on ionization
- Only **unionized form** easily crosses membranes

Transit Time

- Time drug spends in GI tract
- Affects absorption extent

Enzymatic Degradation

- Some drugs degrade in stomach or intestine

Mathematical modeling

- **Differential equations describe:**
 - Rate of dissolution
 - Rate of absorption
 - Drug concentration over time

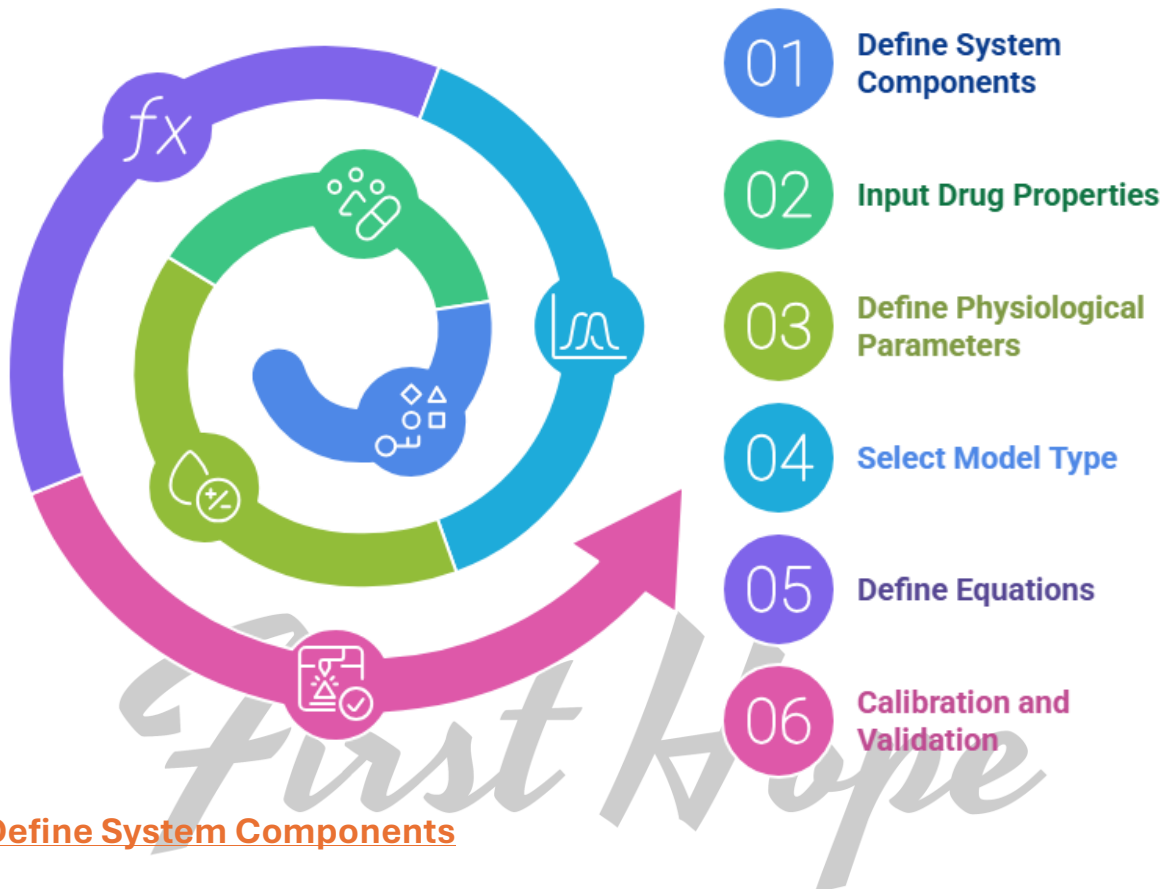
Types of models

- **Compartmental GI models:** Divide GI tract into sections
- **Advanced PBPK models:** Include realistic anatomy and physiology

Model Construction

- Model construction involves building a **mathematical and computational representation of the GI system**.

Steps in Model Construction



A. Define System Components

- Stomach
- Small intestine (duodenum, jejunum, ileum)
- Colon
- **Each segment has:**
 - Different pH
 - Different transit time

B. Input Drug Properties

- Solubility
- Permeability
- pKa
- Particle size

C. Define Physiological Parameters

- GI fluid volume
- Enzyme activity

- Surface area

D. Select Model Type

A. Models

- GI tract divided into compartments
- Each compartment has specific properties

B. PBPK Models

- More detailed
- Include real anatomy and physiology

E. Define Equations

- Dissolution equations
- Absorption rate equations
- Transit equations

F. Calibration and Validation

- Compare model predictions with experimental data
- Adjust parameters if needed

Outcome

- A working simulation that predicts drug absorption profile

Parameter Sensitivity Analysis

- Parameter sensitivity analysis studies how **changes in input parameters affect the model output.**

Purpose

- Identify critical parameters
- Understand model behavior
- Improve reliability

Process

1. Change one parameter (e.g., solubility)
2. Keep others constant
3. Observe effect on absorption

How It Works

- Change one parameter at a time (or multiple)



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