Modeling of complex metallurgical systems using dissipative structures and system dynamics

V P Tsymbal and P A Sechenov
Siberian State Industrial University, 42 Kirova street, Novokuznetsk, 654007, Russia
E-mail: tsymbal33@mail.ru

Abstract. The principles of physical and chemical processes modeling in a column spray-emulsion reactor in the form of dissipative structures are considered, which simplifies greatly the modeling. Comparison of two fundamentally different numerical methods of flow modeling is presented: Smooth Particle Hydrodynamics (SPH) method and method of Adaptive Mesh Refinement (AMR). The advantage of SPH method over the AMR grid methods is the high resolution at a constant number of particles. To solve the problem of simulation, a method similar to the method of smoothed Lagrangian particles was chosen. However, in the problem the mechanisms of interaction between particles, slag, metal, and also particle propagation are simulated. The isolation of dissipative structures made it possible to sharply reduce the dimension of the problem, since at the next higher level in this case, information is used only about the input and output parameters of this structure, complex interactions are closed within the dissipative structure. For the modeling the object-oriented programming language Action Scipt 3.0 was used, which allows the motion, the interaction of particles in a gravity separator to be visualized and animated in real time.

1. Introduction
The object of the study is gas-dynamic, physical and chemical processes in a column spray-emulsion reactor based on the system model of a complex of dissipative structures.

The creation of a continuous steelmaking process was an old dream of metallurgists. A.M. Bigeyev [1] and a number of other researchers considered the existence of separate chambers (zones) for the realization of necessary technological operations as an important and necessary advantage of such a process, along with the absence of intermediate losses of energy and raw materials. However, in connection with the process close to the equilibrium state (and, consequently, low rates of chemical reactions), these chambers turned out to be rather bulky, and the unit as a whole was capital intensive.

In the spray-emulsion reactor due to the transition to the gas suspension and emulsion zone, it was possible to create certain zones (in contrast to the physical chambers discussed above) in the form of dynamic dissipative structures that exist only at the moment of the process in a certain mode [2]. The zone model of a spray-emulsion reactor, includes the following zones (figure 1): 1 – core of the seal, 2 – reactor-oscillator, 3 – connecting channel, 4 – dynamic cushion, 5 – relatively dense gas-slag emulsion, 6 – dissipative gravity separator, 7 – wall layer with a negative (reverse) velocity, 8 – layer of liquid metal.

The most deviated from equilibrium is the zone 6 - the dissipative gravitational separator. Let's consider this zone in more detail.
Figure 1. Zone model of the spray-emulsion reactor.

The dissipative gravitational separator (zone 6) is a sufficiently high layer of froth gas-slag-metallic emulsion suspended above zone 4. This zone occupies the overwhelming part of the column reactor. Due to the influence of the gravitational component and the emulsion velocity in the cross section of the column reactor, separation of the particles takes place depending on their density, size and collisions with other particles. At the same time, the particles of reduced iron, having a density two or three times greater than that of the iron oxide particles, “roll down” to the periphery of the flow and form a wall layer (zone 7). This phenomenon was observed by us on the physical model.

2. Choice of numerical methods

The problem of physical and chemical interaction of the dispersed particles of the charge and the reactions products in the flow of the carrying high-temperature gas has no analytical solution. One of the possible ways to solve it is simulation modeling using the approach similar to the “first principles” method in combination with stochastic modeling. Below we will consider the numerical methods used to simulate two-phase flows.

There are two fundamentally different approaches to numerical methods of flow modeling [3]: Smooth Particle Hydrodynamics (SPH) methods and methods of Adaptive Mesh Refinement (AMR).

The smoothed particle hydrodynamics method is an effective meshless Lagrangian method used to calculate the structure of flows with an unknown free boundary, in particular, high-speed processes in media with a significantly changing topology of simulated objects [4].

In this method, N particles of spherical shape are placed in the simulated physical space, each particle has mass, internal energy, velocity and moves in accordance with the laws of mechanics [5]. Hydrodynamic quantities, such as density and pressure, are defined as the result of the contribution of particles in a certain region [4].

In connection with the fact that the task of describing physical and chemical processes does not have an analytical solution, the method on adaptive meshes, using differential equations in the basis of its solution, can not be applied.
The advantage of SPH method in comparison with the mesh methods of AMR is high resolution at a constant number of particles, while for grid methods it is required to increase the number of calculated points in space in order to refine the results (for example, with a non-uniform flow density).

The disadvantage of SPH method is the finding of an effective method for searching neighbors in the space.

To solve the problem of simulation, a method similar to the method of smoothed Lagrangian particles was chosen. However, in the problem being developed, collisions between particles are taken into account, mechanisms of interaction between particles, slag, metal, and also the particle propagation are simulated. The Monte Carlo method was applied to model the mechanisms of interactions between particles, generation of radius and composition of particles.

3. Isolation of dissipative structures for folding information about the object of research
Isolation of dissipative structures allows the dimension of the problem to be sharply reduced, because at the next higher level, in this case, only the input and output parameters of this structure are used. Complex interactions are closed within a dissipative structure.

In the simulation model under consideration, at a low level (of the floating and interacting particles), the dissipative gravitational separator model (zones 6 and 7) is considered. Zone 5 – relatively dense slag emulsion and zone 8 – a layer of liquid metal, are considered as dissipative structures with input and output parameters.

4. How, and at what level is column gravitational separator simulated?
The program is written in the object-oriented programming language Action Script 3.0, which allows the motion, the interaction of particles in a gravity separator to be visualized and animated in real time.

What objects are allocated and implemented in the program (the appropriate classes are developed)?

The space of the column spray-emulsion reactor is divided into three dissipative structures that interact with each other: a gravitational separator, a slag, and a metal. In this case, for the gravitational separator, as mentioned above, the particle method is used. In this connection, the following objects (classes) are displayed that reflect the physicochemical phenomena in the gravitational separator: condensed particles and gas particles. At the level of dissipative structures, the objects are: the slag below and the metal below.

In turn, the object (condensed particles) is divided into three types: ore, metal and slag.

Let us consider the input-output parameters of each of the selected structures (figure 2).

As it can be seen from figure 2, the input and output objects for each of the allocated structures are particles. At the same time the gravitational separator leads to the formation, collision, melting and formation of new particles. The gas particles formed in the gravity separator together with the initial gas composition are discharged into the gas outlet. And the composition of the gas in it, at this point in time, is determined by the composition of the outgoing gas particles. As a result of the melting of iron ore particles in the gravitational separator, slag particles are formed that can fly to the slag collector or fall into a dense layer of slag. The composition of the dense layer of slag is formed from the slag particles trapped in it, and the composition of the metal is formed from the composition of the metallic particles that have fallen into it.

In dissipative structures, such as slag and metal, internal processes are not considered at the particle level. Only processes occurring at the slag-metal interface (diffusion transition) are described, as a result of which gas, metal and slag particles are formed. The composition of the metal depends on the composition of the metal particles trapped in the collector and the decarbonization rate at the slag-metal interface.
Thus, we obtain a system of interconnected objects. In this case, the most deviated from the equilibrium object – the gravitational separator – is given special attention. It is considered and modeled on the basis of particles. This in turn allows all the required characteristics from the change in the space and time of the composition of the heterogeneous two-phase flow to be studied, and in the composition of the main output product – metal, depending on the constructive and mode parameters.

5. Conclusion
In the paper the object of research is described. The choice of numerical methods for modeling heterogeneous processes in a column reactor is substantiated. It is shown that the isolation of dissipative structures allows the number of connections and calculations of the modeled object to be reduced. The object-oriented programming language Action Script is chosen as a modeling tool. In this connection, the main modeling subobjects are selected and their input and output parameters are shown.

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