Revision of JAERI-QMD for analysis of peripheral nucleus-nucleus collisions

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Abstract
The JAERI quantum molecular dynamics (JQMD) model was improved to reproduce production of projectile-like fragments in nucleus-nucleus collisions by refining the description of reaction mechanisms in peripheral collisions. In the previous version of JQMD, the formulation of the interaction between nucleons was not Lorentz-covariant therefore JQMD adopted supplementary assumptions to inhibit unrealistic phenomena. In the new version (JQMD-2.0), by adopting Lorentz-covariant formulation of nucleon-nucleon interactions, the extra assumptions were eliminated. Fragment production cross sections calculated by JQMD-2.0 combined with a statistical decay model were compared with the experimental data. The comparison shows that fragment production cross sections calculated by JQMD-2.0 are generally in good agreement with the experimental data. In particular, the agreement of the production cross sections for projectile-like fragments underestimated by JQMD are substantially improved.

1. Introduction
For prediction of radiological impact by heavy ions in space and heavy-ion accelerator facilities, nucleus-nucleus reaction models play a fundamental role. Some approaches have been developed and applied to study various nucleus-nucleus reactions. Quantum molecular dynamics [4] is one of such approaches commonly adopted in general-purpose Monte-Carlo radiation transport codes [5][6][7]. JAERI Quantum Molecular Dynamics (JQMD) model is used as the event generator of Particle and Heavy Ion Transport Code System (PHITS) for the dynamical part of nucleus-nucleus reaction simulation. JQMD combined with the statistical decay model GEM [8] was successfully applied to predict fragment production cross sections [9][10][11] and neutron production cross sections [12][13][14]; however, it was suggested that JQMD systematically underestimated heavy fragments [9]. Moreover, Mancusi et al. indicated [15] that Lorentz-covariant treatment of nucleon-nucleon interactions was necessary to reproduce peripheral collisions, in which the stability of nuclei was particularly important to distinguish true nuclear abrasion and spurious nuclear disintegration.

Generally, peripheral collisions are responsible for production of fragments with mass number close to that of target or that of projectile (hereafter referred to as near-target fragments) because in such reactions, small number of nucleons are involved and are knocked-out from the nuclei. In addition, fragment production cross sections increase with decrease in the loss of mass through fragmentation reactions. Therefore production cross sections for near-target fragments are larger than those for lighter fragments and depend on the description of peripheral collisions. Because of the large production cross sections, near-target fragments are important in radiation safety of accelerator operation and cancer therapy. Substantial portion of remanent dose is attributed to decay radiation of near-target fragments; however, there were some technical challenges in simulating near-target fragment production. For the first thing, nuclei were sometimes spuriously disintegrated even without interacting with other nuclei owing to the instability inherent to the description of nucleon-nucleon interactions. In this case, model cannot distinguish the spurious decay and peripheral collisions. Secondly, nucleon-nucleon interactions
at the nuclear surface and those in dense nuclear medium are different in a sense that Pauli-blocking is strong in the depth of nuclei and thereby interactions between nucleons are suppressed.

In this study, we revise the description of reaction mechanisms in JQMD to simulate peripheral collisions accurately. In association with the description of the interaction between nucleons, the complementary assumptions adopted in JQMD were also revised. Fragment production cross sections calculated by the revised JQMD (JQMD-2.0) were compared with experimental data of earlier studies for benchmarking.

2. Methods

JQMD-2.0 was developed as an upgrade of JQMD, whose details are provided elsewhere [7]. As pinpointed previously [15], the description of nucleon-nucleon interactions was not Lorentz-covariant in JQMD, therefore nuclei were spuriously excited or disintegrated occasionally during time evolution in the center-of-mass frame. Lorentz-covariant equation of motion adopted in JQMD-2.0 is described as follows;

\[ \dot{r}_i = \frac{p_i}{2p_i^0} + \sum_j^N \frac{m \partial \langle \hat{V}_j \rangle}{p_j^0 \partial p_i}, \]

\[ \dot{p}_i = -\sum_j^N \frac{m \partial \langle \hat{V}_j \rangle}{p_j^0 \partial r_i}, \]

\[ p_i^0 = \sqrt{p_i^2 + m^2 + 2m \langle \hat{V}_i \rangle}, \]

where \( r_i \) is the spatial coordinate of the centroid of the \( i \)-th nucleon, \( p_i \) is the momentum of the \( i \)-th nucleon, \( m \) is the rest mass of nucleons, \( \langle \hat{V}_j \rangle \) is the potential of \( j \)-th particle, and \( N \) is the number of particles in the system. In both JQMD and JQMD-2.0, the potential term of the Hamiltonian \( V \) is a sum of the Skyrme-type force term, Coulomb interaction term, and symmetry term. The potential \( V_i \) is described by the following formula;

\[ V_i = \frac{1}{2} A \langle \rho_i \rangle + \frac{1}{1 + \tau \rho_i^e} \langle \rho_i \rangle^\tau + \frac{1}{2} \sum_j c_i c_j e^2 \left| \frac{R_i - R_j}{4L} \right| \text{erf} \left( \frac{|R_i - R_j|}{\sqrt{4L}} \right) + \frac{C_s}{2\rho_s} \sum_j (1 - 2|c_i - c_j|) \rho_{ij}, \]

where \( A \) is a Skyrme force parameter (= -219.4 MeV), \( \rho_s \) is the saturation density (=0.168 fm\(^{-3}\)), \( \langle \rho_i \rangle \) is the overlap integral of wave packets between the \( i \)-th nucleon and all the other nucleons, \( B \) is another Skyrme force parameter (= 165.3 MeV), \( \tau \) is 4/3, \( c_i \) is 1 for protons and 0 for neutrons, \( e \) is the elementary charge, \( R_i \) denotes the position of \( i \)-th nucleon, \( L \) is the square of the width of wave packet representing nucleons (= 2 fm\(^2\)), \( C_s \) is the symmetry energy parameter (= 25 MeV), and \( \rho_{ij} \) is the overlap integral of wave functions of the \( i \)-th and \( j \)-th nucleons. The potential description of JQMD-2.0 was inherited from previous JQMD without any modifications. Using the new equation of motion, nuclei at the ground state almost always stay stable over a typical reaction period of 150 fm/c.

Moreover, the medium effects on nucleon-nucleon scattering cross sections were modified. Previously, the cross sections were calculated with the modified version of the Cugnon’s formula [16,17], which assumed that cross sections were reduced by Pauli blocking. In the new version, on the other hand, the cross sections in the free space were adopted in case the impact parameter was larger than 60% of maximum impact parameter \( b_{\text{max}} \). Here, \( b_{\text{max}} \) was estimated by carrying out reaction simulation using different random number seeds with sweeping the impact parameter from zero. The impact parameter at which inelastic reaction probability reached below 20% was defined as the maximum impact.
In addition to the above-described improvements on the physical reaction mechanisms, supplementary algorithms were revised accordingly. To disregard spurious excitation in JQMD, the simulated events in which the excitation energies of target and projectile were lower than the threshold calculated using Eq. 2:

\[ E_{\text{ex}} = 0.3 \times A, \]  

where \( A \) is the mass number of the nucleus, were rejected and reaction simulation was started afresh. This formulation was reasonable in a sense that the spurious excitation energy was increased with the size of nuclei in JQMD; however, in case of \(^{12}\text{C}(^{12}\text{C},x)\) reaction for example, peripheral collision events in which 4 MeV of excitation energy was given to target and projectile were accepted as true reaction events. In this case, projectile and target just pass by without abrading each other reality. Because spurious excitation was substantially suppressed in JQMD-2.0, the separation energy of proton, neutron, and alpha was adopted as the excitation energy threshold as calculated by Eq. 3:

\[ E_{\text{ex}} < \min(S_n, S_p + V_p, S_\alpha + V_\alpha). \]

The impact parameter was sampled from zero to a threshold calculated by Eq. 4 in JQMD to cut off spurious reactions:

\[ b_{\text{max}} = 1.15 \times \left( A_t^{1/3} + A_p^{1/3} \right) - 0.4 \text{ fm}, \]

where \( A_t \) is target mass number and \( A_p \) is projectile mass number. On the other hand, impact parameter was cut off intrinsically in JQMD-2.0, which means that projectile and target stay without losing nucleons in reactions at extremely large impact parameters. In this case, reaction simulation was started afresh after newly sampling the impact parameter. It should be mentioned that impact parameter sampling algorithm in central collisions was also revised. In both JQMD and JQMD-2.0, energy conservation was occasionally violated owing to numerical integration of time evolution. If the deviation of total energy at the beginning and that at the end of reaction was small, the energy was balanced by scaling the excitation energy of the reaction residues. In case the total energy could not be balanced by the scaling of excitation energy (hereafter referred to as a non-energy-conserving event), the event was rejected and reaction simulation was started from the beginning. In JQMD, the impact parameter was newly sampled at random after the rejection; however, central collision events, in which energy balance was often violated, were considerably rejected by this scheme. As a result, the impact parameter sampling was biased. Therefore, JQMD-2.0 restarted reaction simulation with the same impact parameter in the non-energy-conserving events.

Despite the revision on the description of nucleon-nucleon interactions, nuclei were occasionally excited or disintegrated spuriously owing to their intrinsic instability. To avoid such spurious reactions, time evolution of initialized nuclei was followed for a time scale of 150 fm/c to check if spurious excitation or disintegration were observed. This check was performed if the impact parameter was larger than \( (b_{\text{max}} - 4) \text{ fm}, \) otherwise stability check was not performed because reaction was not sensitive to stability of the nuclei. The further details on JQMD-2.0 are provided elsewhere [18].

### 3. Results and Discussion

Typical fragment production cross sections calculated using PHITS-JQMD-2.0 are compared with experimental data [19] in Fig. 1. JQMD-2.0 predicts the increase in fragment yields by a factor of 4 in the range from \( Z=20 \) to \( Z=25 \) accurately owing to the reasonable treatment of peripheral collisions. On the other hand, the cross section calculated by JQMD is almost constant; therefore the yields for
fragments with large Z are systematically underestimated. It is also suggested that the odd-even effect is overestimated by both JQMD and JQMD-2.0 although the odd-even effect was considered only in the statistical decay phase.

Comparison of fragmentation cross sections in higher energy is shown in Fig. 2. Isotopic fragmentation cross sections of $^{59}$Co($^{12}$C,x) reactions measured at 3650 MeV/nucleon [20] are compared with the cross sections calculated using the old JQMD and JQMD-2.0. The cross sections calculated by JQMD-2.0 agree with experimental data within a factor of 2 except those of $^{24}$Na and $^{59}$Fe, on the other hand, JQMD generally underestimates cross sections and the deviation systematically increases with increase in product mass above $A=40$. In this region, the production cross section tends to increase with mass by one order of magnitude at maximum but the production cross section calculated using JQMD cannot follow this trend, similar to the cross section in Fig. 1. Fig. 2(a) shows that fragmentation cross sections vary with isotopic identity by orders of magnitude; however, JQMD-2.0 can predict production cross sections accurately regardless of the absolute magnitude of cross sections as shown in Fig. 2(b). Because soft neutron-proton exchange mechanism is necessary to simulate $^{59}$Co($^{12}$C,x)$^{59}$Fe reactions, the improvement of JQMD-2.0 is not effective. On the other hand, the improvement is effective for production of fragments with mass number close to that of the target (e.g., $^{59}$Co($^{12}$C,x)$^{58}$Co).

By taking advantage of JQMD-2.0, accuracy of $\beta^+$-emitter production calculation, which is useful for dose monitoring in heavy-ion radiotherapy, can be improved. Fig. 3 shows depth profiles of $^{11}$C and $^{10}$C measured in a thick PMMA (Poly Methyl MethAcrylate) target irradiated with 266
Fig. 3: Depth profile of $^{10}$C and $^{11}$C produced in a thick PMMA target bombarded by 266 MeV/nucleon $^{12}$C ion beam.

MeV/nucleon $^{12}$C ions [21]. $^{11}$C and $^{10}$C are produced dominantly by fragmentation of $^{12}$C in PMMA induced by projectiles. Production is still underestimated by JQMD-2.0; however, production is increased by the upgrade of JQMD, which indicates that precise treatment of peripheral collisions is an important factor of this calculation. Although some portion of $^{11}$C production is attributed to secondary neutrons, protons, and alphas, fragment yield near the projectile range is accumulation of projectile fragments produced along the paths and they are underestimated. This means that production of primary ion fragment is still underestimated. In contrast, the fragments along the projectile path (between the target surface and 90 mm of depth) are target fragments produced at higher energies. The underestimation of fragment yields in this region indicates that further improvements effective for high energy reactions are still necessary.

4. Conclusion

JAERI quantum molecular dynamics model was improved to accurately reproduce fragment production. Production of target-like fragments, which are generally attributed to peripheral collisions is predicted by JQMD-2.0 at higher accuracy compared to JQMD. Increase in fragmentation cross sections with increase in product mass near the target mass is well reproduced by JQMD-2.0 in the relativistic energy range. This improvement is beneficial for the applications such as dosimetry in heavy ion cancer therapy and remanent dose prediction in accelerator facilities.

Because the CPU time spent per reaction event was almost doubled by this improvement, the algorithm should be optimized in future upgrade. JQMD-2.0 has been incorporated to PHITS Ver. 2.76 and later.

References


